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# LabSolutions LCMS

## Operators Guide

Read the instruction manual thoroughly before you use the product.
Keep this instruction manual for future reference.

# Introduction

## Read this Instruction Manual thoroughly before using the product.

Thank you for purchasing Shimadzu analytical instrument workstation “LabSolutions LCMS” (hereafter referred to as “the software” or “LabSolutions”).

This manual describes the procedures for operating this product. Read this manual thoroughly before using the product and operate the product in accordance with the instructions in this manual.

Also, keep this manual for future reference.

This manual assumes that the reader is knowledgeable of basic operations of Windows. For the operation of Windows, refer to the instruction manual that comes with that product.

# Important

- If the user or usage location changes, ensure that this Instruction Manual is always kept together with the product.
- If this manual is lost or damaged, immediately contact your Shimadzu representative to request a replacement.
- To ensure safe operation, contact your Shimadzu representative of product installation, adjustment, or re-installation (after the product is moved), or repair is required.


Original version is approved in English.

# Notice

- Information in this manual is subject to change without notice and does not represent a commitment on the part of the vendor.
- Any errors or omissions which may have occurred in this manual despite the utmost care taken in its production will be corrected as soon as possible, although not necessarily immediately after detection.
- 
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  Adobe, Adobe logo and Adobe Reader are trademarks or registered trademarks of Adobe Systems Incorporated in the United States and/or other countries.
  Other company names and product names mentioned in this manual are trademarks or registered trademarks of their respective companies. The TM and ® symbols are omitted in this manual.
- Microsoft® Windows® Operating System is referred to as “Windows”.
- LabSolutions is registered trademarks of Shimadzu Corporation in the United States and Europe (Office for Harmonization in the Internal Market).
- Replacement parts for this product will be available for a period of seven (7) years after the product is discontinued. Thereafter, such parts may cease to be available. Note, however, that the availability of parts not manufactured by Shimadzu shall be determined by the relevant manufacturers.

# Instruction Manuals

## ■ List of Instruction Manuals

| Name | Content |
|---|---|
| Getting Started Guide | This manual follows an actual data acquisition procedure to describe basic methods of operation for first-time users. Read this manual to learn basic operations of the software. |
| Operators Guide | This manual describes overall operations and handy functions in more details, such as the software's system configuration, data analysis, batch processing, confirmation of data acquisition results, and report functions. |
| System Users Guide | This manual describes system administration and data management of the software. Refer to this manual as necessary. |
| Installation & Maintenance Guide | This manual describes installation and maintenance of the software. |
| Data Acquisition & Processing Theory Guide | This manual describes peak detection and quantitation of sample components.<br>Refer to this manual as necessary. |
| Help | Clicking the on-screen [Help] button or pressing the [F1] key displays a description of on-screen parameters, answers to specific questions or solutions to various problems. Also, clicking the [Help] button on the error message window displays the details of the error or solutions to the error. Refer to Help before contacting us. |

## ■ Indications Used in Instruction Manuals

Cautions and Notes are indicated using the following conventions, and the following symbols are used in this manual:

| Indication | Meaning |
|---|---|
| ⚠ CAUTION | Indicates a potentially hazardous situation which, if not avoided, may result in minor to moderate injury or equipment damage. |
| **NOTE** | Emphasizes additional information that is provided to ensure the proper use of this product. |
| ☞ Reference | Indicates the location of related reference information. |
| [ ] | Indicates the names of buttons, menu options, setting options, windows/sub-windows, and icons that are displayed in a window.<br>Example: Click [OK]. |

# Warranty

Shimadzu provides the following warranty for this product.

**1. Period:**

Please contact your Shimadzu representative for information about the period of this warranty.

**2. Description:**

If a product/part failure occurs for reasons attributable to Shimadzu during the warranty period, Shimadzu will repair or replace the product/part free of charge. However, in the case of products which are usually available on the market only for a short time, such as personal computers and their peripherals/ parts, Shimadzu may not be able to provide identical replacement products.

**3. Limitation of Liability:**

1) In no event will Shimadzu be liable for any lost revenue, profit or data, or for special, indirect, consequential, incidental or punitive damages, however caused regardless of the theory of liability, arising out of or related to the use of or inability to use the product, even if Shimadzu has been advised of the possibility of such damage.
2) In no event will Shimadzu's liability to you, whether in contract, tort (including negligence), or otherwise, exceed the amount you paid for the product.

**4. Exceptions:**

Failures caused by the following are excluded from the warranty, even if they occur during the warranty period.

1) Improper product handling
2) Repairs or modifications performed by parties other than Shimadzu or Shimadzu designated companies
3) Product use in combination with hardware or software other than that designated by Shimadzu
4) Computer viruses leading to device failures and damage to data and software, including the product's basic software
5) Power failures, including power outages and sudden voltage drops, leading to device failures and damage to data and software, including the product's basic software
6) Turning OFF the product without following the proper shutdown procedure leading to device failures and damage to data and software, including the product's basic software
7) Reasons unrelated to the product itself
8) Product use in harsh environments, such as those subject to high temperatures or humidity levels, corrosive gases, or strong vibrations
9) Fires, earthquakes, or any other act of nature, contamination by radioactive or hazardous substances, or any other force majeure event, including wars, riots, and crimes
10) Product movement or transportation after installation
11) Consumable items
    Note: Recording media such as CD/DVD-ROMs are considered consumable items.

* If there is a document such as a warranty provided with the product, or there is a separate contract agreed upon that includes warranty conditions, the provisions of those documents shall apply.
* Warranty periods for products with special specifications and systems are provided separately.
* The license cannot be reissued if you lose the license certificate or the USB dongle.

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# 1 What is LabSolutions?



This software is a workstation for high-performance liquid chromatograph mass spectrometer systems (hereafter referred to as “LCMS”).

It enables control of LC and MS units from a personal computer (PC), and perform tasks such as chromatogram data acquisition, data analysis, report generations, and data management.

This chapter introduces the main features and functions of the software.

## 1.1 Features

### ■ Abundant Functions with Simple Operations

#### Assistant Bar

Click an icon on the assistant bar to change the display to the target operation sub-window. Icons displayed on the assistant bar can be customized to support a wide variety of operations.

#### Data Explorer

The file content is displayed by dragging-and-dropping the file from the [Data Explorer] sub-window onto the target sub-window.

Outstanding file management functions are provided for copying, moving, and deleting files, and for browsing the history information of files.

#### Batch Table Wizard

Batch Tables for sequential analysis of multiple samples are easily set by following the on-screen instructions.

#### Data Browser

The [Data Browser] window enables import and browsing of up to 64 data files.

#### Quant Browser

The [Quant Browser] window enables browsing of multiple quantitative calculation results that were acquired using the same method.

### ■ Enhanced Identification and Quantitative Processing Functions

This software supports a variety of identification methods such as window, band, spectrum similarity, absolute retention time and relative retention time. There are 6 different quantitative calculation methods that include the external and internal standard methods, and 7 types of calibration curves such as linear and exponential.

### ■ Highly Flexible Report Format

The report format function offers a high degree of flexibility by allowing creation of reports such as chromatograms, calibration curves, quantitative results, summary reports, and data analysis reports.

This software has a substantial selection of pre-installed report format templates, making it easier to create the desired report format.

## ■ Enhanced GLP/GMP Support Functions

The software contains functions that provide sure and efficient compliance with reliability requirements mandated in various regulations such as GLP/GMP and FDA 21CFR Part 11.

### FDA 21 CFR Part11 Compliance

The electronic record and electronic signature functions of this software comply with the requirements of 21 CFR Part 11.

Information such as data measurement methods, schedules, date/time, operator name, and chromatograms can all be saved at once, and human and machine readable data can be saved together as required for compliance with Part 11.

**NOTE**

When used in combination with the optional CLASS-Agent Manager, this software meets the Part 11 requirements for electronic records and electronic signatures for review, approval and long-term storage of data.

### User Administration

The Shimadzu User Authentication Tool administers users on the Shimadzu network. Account policies such as the minimum number of characters in passwords, password update interval, and permitted number of entry attempts are set to prevent illegal accessing.

### System Administration

The software is also has an audit trail function and log browser function for sure and efficient operation of the system. The audit trail function records a history of changes to instrument parameters and data processing parameters, and the log browser function allows for a quick search of the system operation history.

The functions have been efficiently arranged to allow the extensive range of functions to be easily put to effective use.

# 1.2 Basic Knowledge

The software is comprised of the following programs:

| Program Name | Contents |
|---|---|
| [Realtime Analysis] program | Used to enter the data acquisition parameters and acquire the data. |
| [Offline Editor] program | Allows other method files and batch files to be edited during data acquisition, and can register a single or batch data acquisition to the data acquisition queue. |
| [Postrun Analysis] program | Analyzes the acquired data to detect the peaks of chromatogram and perform quantitative calculations on these peaks. |
| [Browser] program | Allows importing and browsing of up 64 data files for [Data Browser] window or 1024 data files for [Quant Browser] window. |
| [Security Policy Settings] program<br>[User Administration] program | Administers the system security and user accessibility to the software. |

Each of these programs are opened from the [LabSolutions Main] window.

This section describes how to open the [LabSolutions Main] window and the functions contained therein.

## ■ Open the [LabSolutions Main] Window

The (LabSolutions) icon is displayed on the Desktop.

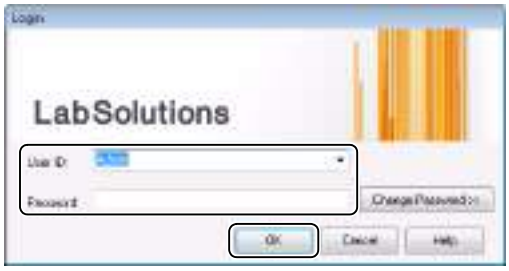
**1** **Verify that the [LabSolutions Service] icon in the Systray on the Taskbar displays a green chromatogram.**


**NOTE**

A yellow chromatogram in the [LabSolutions Service] icon indicates that the software is still initializing. Wait for the chromatogram to turn green. A red chromatogram in the [LabSolutions Service] icon indicates that an error has occurred. Restart the PC.

**2** **Double-click the (LabSolutions) icon on the Desktop.**

**3** **Select a registered user ID from the [User ID] list, enter the [Password] and click [OK].**




**NOTE**

Select [Admin] in the [User ID] list for the first login to the system, and click [OK].

The [LabSolutions Main] window opens.

## ■ [LabSolutions Main] Window

The [LabSolutions Main] window displays an icon bar and a box for selecting a specific operation of a selected icon.

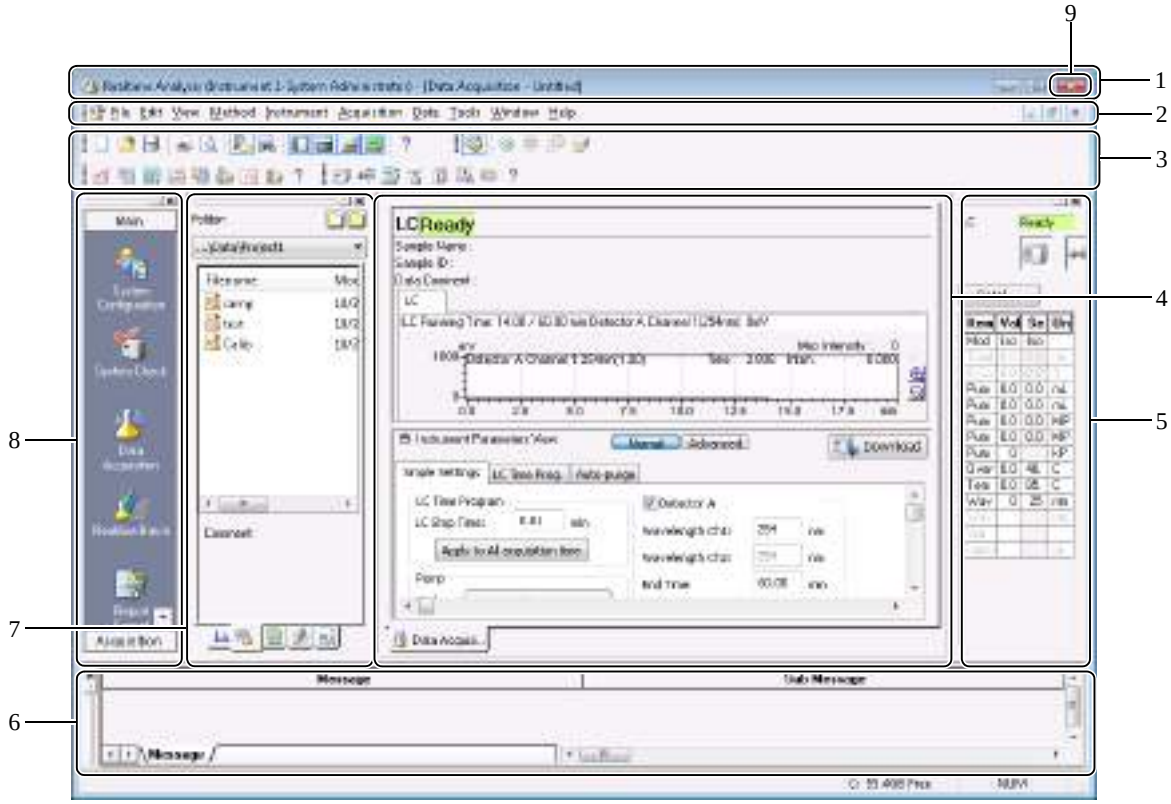
| Icon Bar | Explanation |
|---|---|
|  | Click this icon to display icons for each of the instruments connected to the PC. Tables or icons can be displayed in the [Instruments] sub-window. Right-click on the [Instruments] sub-window, and click [Table View] from the displayed menu. The display changes to the table display.<br>Double-click an instrument icon to open the [Realtime Analysis] program. The [Realtime Analysis] program is used to set the data acquisition parameters, acquire data and check the operating status of the instruments.<br><br>[Table View]<br>  |
|  | Click this icon to open either the [Postrun Analysis] program to analyze data or the [Browser] program to display chromatograms and statistical calculation results from multiple data files. |
|  | Click this icon to perform system administration functions related to the security policy, user administration, system settings, and validation. |
|  | Click this icon to select a specific PDF formatted Instruction Manual or the Help files. |

**NOTE**

- Depending on the specific user's rights, the program icons in the icon bar of the [LabSolutions Main] window are sometimes not displayed or are disabled.
- Click  at the top right corner of the sub-window to close the [LabSolutions Main] window.

## ■ Basic Functions of the [Realtime Analysis] and [Postrun Analysis] Programs

This section describes the [Data Acquisition] window in the [Realtime Analysis] program.




| No. | Explanation |
|---|---|
| 1 | The title bar displays the name of the currently running program, window name, currently loaded file name, logged in user name, and other information. |
| 2 | The menu bar displays the menus that are enabled according to the current window and rights of the logged in user. |
| 3 | The toolbar displays icons for frequently used menu items and icons for operating analytical instrument. |
| 4 | Different sub-windows such as [Data Acquisition] and [Realtime Batch] can be displayed in this section of the [Realtime Analysis] program.<br>Sub-windows such as [Data Analysis], [PDA Data Analysis], [Calibration Curve], and [Report] are displayed in the [Postrun Analysis] program. Use the tabs under each sub-window or the icons in the assistant bar to change the displayed window. |
| 5 | The [Instrument Monitor] displays the status of the instruments and the parameter settings. |
| 6 | The [Output Window] displays a history of data acquisition operations and error messages that occur. |
| 7 | The [Data Explorer] sub-window displays the currently selected folder with the project file types (extensions) selectable from the lower tabs. The content of files is displayed by dragging-and-dropping the file in the [Data Explorer] sub-window onto the data analysis sub-window. |
| 8 | The assistant bar displays icons for the frequently used data acquisition operations. Click an icon on the assistant bar to change the data analysis sub-window. Icons displayed on the assistant bar can be customized to support a wide variety of operation flows. |
| 9 | Click  to exit the program. |

# 1.3 File Formats

The software uses the following file formats to handle acquired data and related information:

- Method files
- Data files
- Report format files
- Batch files
- UV spectrum files
- Other files

This section describes each of the file formats.

## 1.3.1 Method Files

Method files store information such as instrument parameters and data processing parameters.

The file extension for method files is ".lcm".

Method files store the following information.

| Stored Information | Explanation |
|---|---|
| System Configuration Information | System configuration information is saved in the method files to allow for review of the instrument parameters. |
| Instrument Parameters | This information includes the instrument parameters for each instrument and also the baseline evaluation results. |
| Data Processing Parameters | Calibration curve information, column performance parameters, QA/QC parameters, peak integration parameters, identification parameters, quantitative parameters, and Compound/Group Tables are all saved in the method file. |
| Sub-Window Properties | The chromatogram XY range setting, whether the status bar is displayed or hidden, etc. are also saved in the method file. |

## 1.3.2 Data Files

The software stores the method files, batch files and report format files, chromatogram data, and quantitation results in a single data file. This is called an "All-In-One" structure and, since the data acquisition and analysis parameters are referenced from the same data file, it ensures the traceability of data.

The file extension for data files is ".lcd".

**NOTE**

- The report formats are also saved to the data file. Click [Data Report] on the [File] menu, then select [Print] to print the acquisition results of the currently loaded data file according to the report format stored with that data.
  The report format can be edited by clicking the [Data Report] icon in the [Data Analysis] assistant bar to display the [Report] window. Click [Save Report Format File As] on the [File] menu to save the edited format for use with other data reports.
- When postrun analysis is performed on chromatogram data, the new data processing parameters are saved to the data file. [Apply to Method] on the [Data Analysis] assistant bar or [PDA Data] assistant bar must be clicked to save the parameters and allow them to be applied to other chromatogram data.

**Reference**

Refer to *"4.7 Save (Export) to Method Files" P.126* for more information.

## 1.3.3 Report Format Files

Items such as pictures or logos and placeholders for chromatograms, results and etc., are pasted into the blank format and it is saved for future printing of data acquisition results.

The file extension for report format files is ".lsr".

If a report format file is set at the time of data acquisition or postrun analysis, the results can be immediately printed according to that format.

**Reference**

Refer to *"7 Report Function" P.245* for information on how to set the batch file.

## 1.3.4 Batch Files

Data such as sample information and quantitative calculation conditions, are saved to a batch file during sequential measurement of multiple samples.

The item displayed in the Batch Table and the overall batch processing parameters are also saved to the batch files.

The file extension for batch files is ".lcb".

**Reference**

Refer to *"3 Realtime Batch" P.43* for information on how to set the batch file.

## 1.3.5 UV Spectrum Files

The software uses the JCAMP format with the file extension of ".jcm" for the UV spectrum file.

When peak identification using the similarity of UV spectra is performed, jcm files are included in the Compound Table as standard spectrum.

The ".jcm" files can also be registered as spectra to the UV library files.

## 1.3.6 Other Files

The software uses the following files in addition to those described above.

| File Name | Contents |
|---|---|
| LCMS Tuning File | These files store the conditions used to perform instrument adjustment (tuning) and the tuning results. The file extension is ".lct". |
| UV Library Files | These files contain multiple UV spectrum data. They are used to perform library searches on the spectrum information for unknown samples.<br>The file extension is ".llb". |
| MS Library Files | These files contain multiple MS spectrum data. They are used to perform library searches on the spectrum information for unknown samples.<br>The file extension is ".lib". |
| Browsing Files | These files store information such as compound information displayed in [Quantitative Results View] and the names of method and data files loaded in the [Quant Browser] window.<br>The file extension is ".lcq". |
| Layout Files | These files store information such as data file names and display layouts loaded in [Data Browser].<br>The file extension is ".lyt". |
| System Configuration Files | These files hold the link information for the PC and analytical instruments, names of the instruments that make up the system, and information on consumables. These file names are not used for regular operations. |
| PDF Files | These files contain electronic versions of printed reports.<br>These files are a generic format that satisfies the requirement of human readable data, and are used when registering and managing the data acquisition result reports in a database. |

# 2 Data Acquisition

This chapter describes the basic flow of operations from entrance of the data acquisition parameters to the performance of a single run data acquisition on the LCMS.

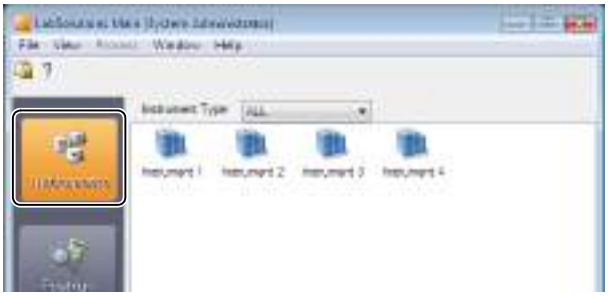


## 2.1 [Data Acquisition] Window

Two views of the [Data Acquisition] window are available, the [Chromatogram View] is used to display chromatograms and instrument status information and the [Instrument Parameters View] is used to display the parameters set for each instrument.

### 2.1.1 Open the [Data Acquisition] Window

**1** **Click the**  **icon.**



**2** **Select and double-click the instrument that will be used for data acquisition.**

The [Realtime Analysis] program opens.

## 3 Click the (Data Acquisition) icon on the [Main] assistant bar.

**NOTE**

If the (Data Acquisition) icon is not displayed, click [Main] on the title of the assistant bar.

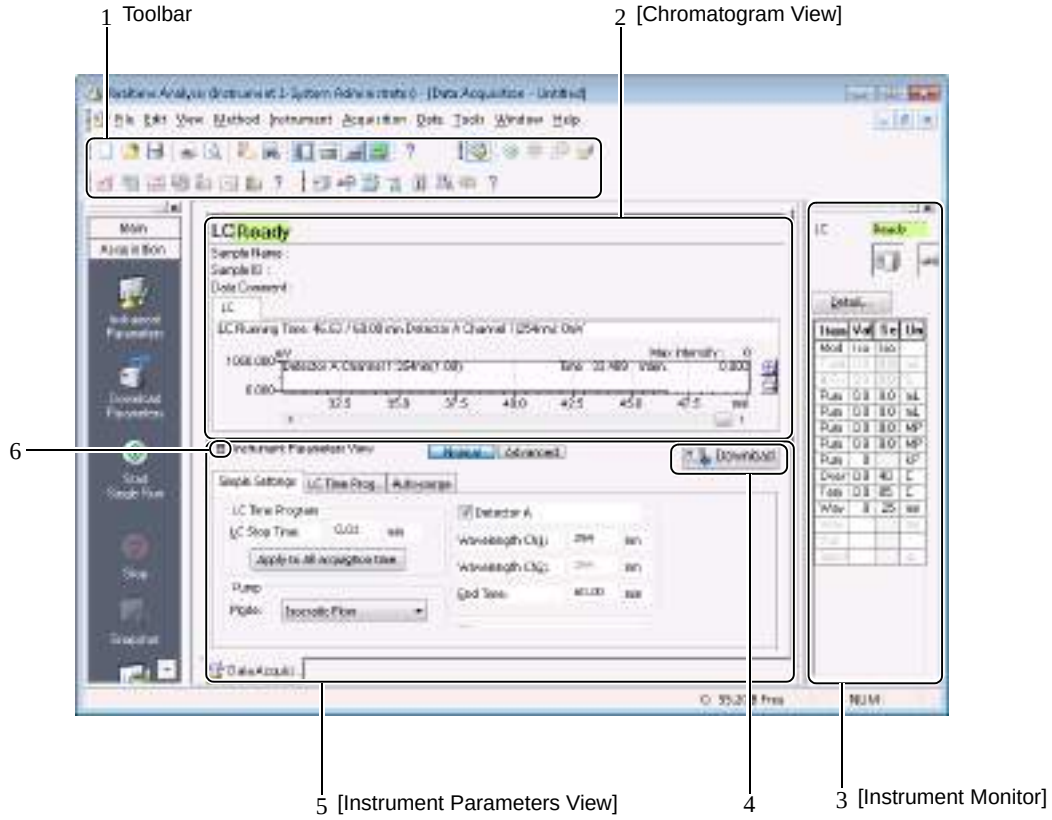
## 4 Ensure that [Ready] is displayed in the [Data Acquisition] window.


**NOTE**

If [Not Connected] is displayed on the status display, refer to "3 System Configuration" in the Installation & Maintenance Guide.

## 2.1.2 [Data Acquisition] Window Description

This section describes how to view and use the [Data Acquisition] window.




| No. | Explanation |
|---|---|
| 1 | Displays the [Standard] toolbar, [Data Acquisition] toolbar, [Instrument Control] toolbar, [LC Control], and [PDA Control] toolbar. |
| 2 | Displays chromatograms and the instrument status curves.<br>A [PDA] tab is displayed when a PDA is configured.<br>An [MS] and [ALL] tab are displayed when an MS is configured.<br>**Reference**<br>Refer to *"2.3.1 Monitor the Chromatograms and Instrument Status Curves" P.23* to display the status information of instruments. |
| 3 | Displays the instrument status and parameter settings. |
| 4 | Click Download to transfer the data acquisition settings set in [Instrument Parameters View] to the analytical instrument.<br>**Reference**<br>Refer to *"2.2.5 Analytical Instrument Startup" P.22* for details. |
| 5 | Displays the instrument parameters for data acquisition.<br>In the [Normal] sub-window, the main data acquisition parameters are set on the [MS], [Simple Settings] and [LC Time Prog.] tabs.<br>In the [Advanced] sub-window, a tab for each configured instrument module is displayed so that data acquisition parameters can be set in more detail. |
| 6 | Switches between the full screen and normal display. |

# 2.2 Enter Data Acquisition Parameters

Enter the data acquisition parameters in [Instrument Parameters View].

The parameters are saved to the method file and used to perform data acquisition.

This section describes the operations in the [Instrument Parameters View] .

## 2.2.1 Switch Between the Displays of Instrument Parameters View

[Instrument Parameters View] has two sub-windows, [Normal] and [Advanced].

In the [Normal] sub-window, the main data acquisition parameters are set on the [MS], [Simple Settings] and [LC Time Prog.] tabs. In the [Advanced] sub-window, a tab for each configured instrument module is displayed so that data acquisition parameters can be set in more detail.

This section describes how to set the data acquisition parameters and create a method file.

**1** **Click [Normal] to open the [Normal] sub-window.**

## 2.2.2 Set the LC Instrument Parameters

This section describes how to set the LC instrument parameters on the [Simple Settings] and [LC Time Prog.] tabs.

**1** **Click the [Simple Settings] tab and enter the data acquisition parameters.**

Set the [LC Stop Time], pump flow rate and initial concentration for gradient systems, oven temperature, detector wavelength and other parameters.

- Enter the data acquisition time from one sample injection to the next sample injection at [LC Stop Time].
- Click [Apply to All acquisition time] to set the [End Time] for each detector to the same value as [LC Stop Time].
- Deselect [Oven] when the oven is not used.

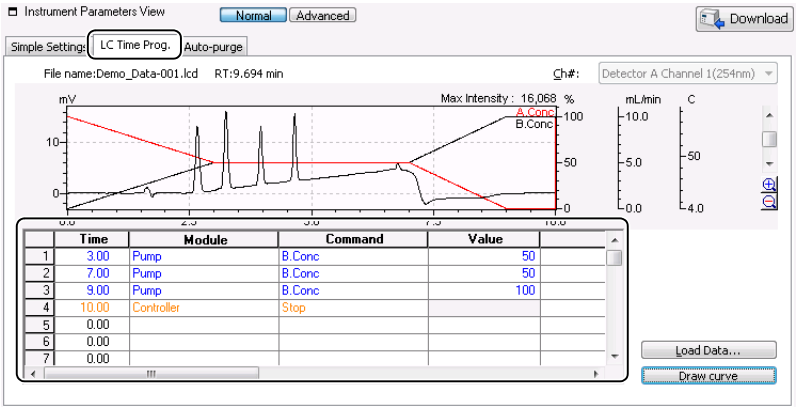
**NOTE**

- To switch the detector lamp off, make this setting on the respective detector in the [Advanced] sub-window.
- The MS detector measurement time is displayed on the [Simple Settings] tab, but it cannot be edited. Set the MS detector measurement time on the [MS] tab.

- The [Auto-purge] tab is displayed when an auto-sampler is used.
  Refer to *"2.3.2 Auto-Purge the Pump and Autosampler" P.27* for details.
- If a new method file is made and the rack set at [Sample Rack] on the [Autosampler] tab does not match the actual rack in use, an error message is displayed and data acquisition cannot be started.
  Click [Detect Rack] on the [Autosampler] tab in the [Advanced] sub-window to correct the rack selection.

**2** **Click the [LC Time Prog.] tab, and enter the concentration gradient conditions.**

When switching the concentration gradient or valve during data acquisition, set [Time], [Unit], [Command], and [Value] for the time program. Clicking [Draw Curve] plots the time program gradient condition settings on the graph.

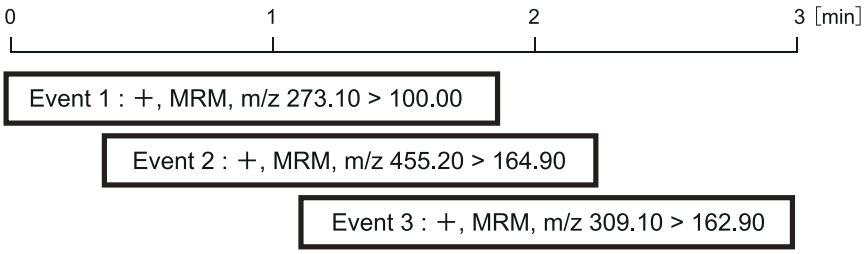



**NOTE**

The time entered in the [Time] column of the time program corresponds to the time elapsed since the start of analysis. Enter a value of at least 0.01 min.

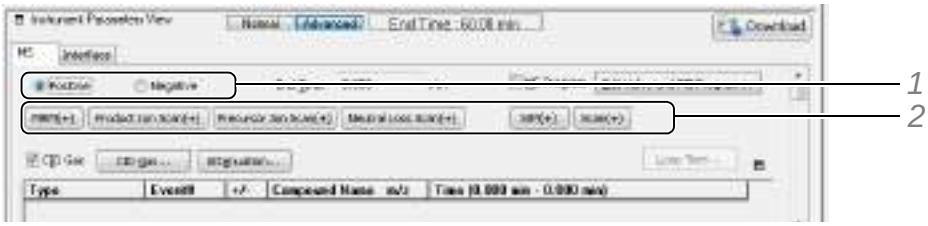
## 2.2.3 Set the MS Instrument Parameters

This section describes how to create events and specify settings on the [MS] tab. This instrument keeps changing MS conditions within the same data acquisition process. Each individual MS condition is called an "event," and polarity can be set to each event. When multiple events are registered, the next event is switched to after the "event time" set for each event has elapsed. When the last event is carried out, gain tothe first event is returned to. (In the case of 1 [min] in the example in the figure below, Event 1 → Event 2 → Event 1, and in the case of 2 [min], Event 2 → Event 3 → Event 2, and so forth) The total time required to execute a series of concurrent events is called loop time.



## 1 Click the [MS] tab.

## 2 Select the polarity and data acquisition mode for the event to add.




1 Select the polarity of the event to set.
2 Click the button for the event's data acquisition mode.
The event is now added to the Event Table.

**NOTE**

The button name for the data acquisition mode changes depending on the selected polarity. When [Positive] is selected, the button name includes a plus symbol, such as [MRM(+)] or [Product Ion Scan(+)].

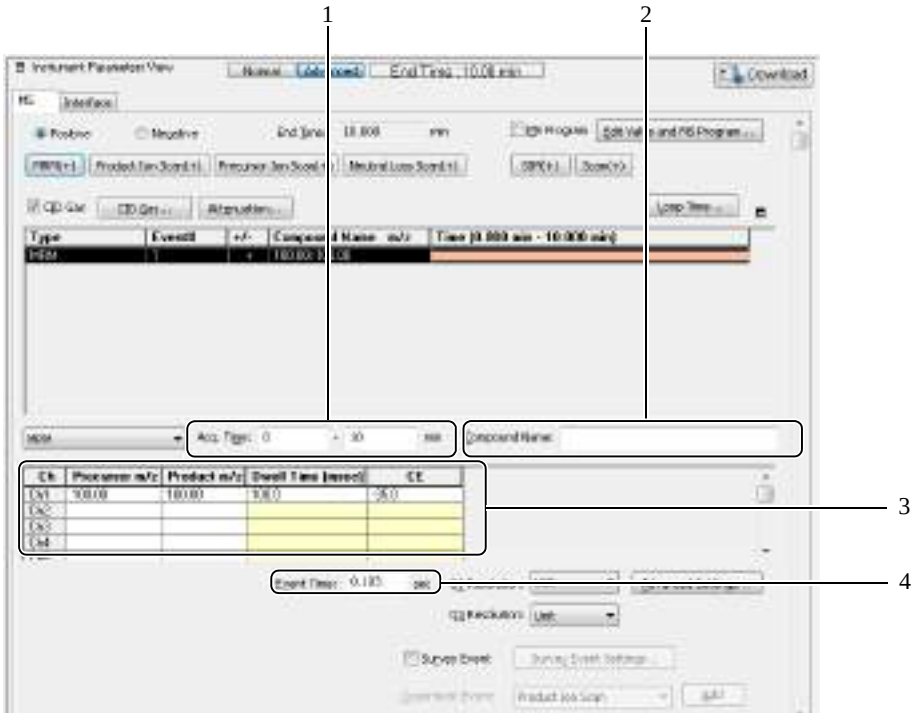

| No | Explanation |
|---|---|
| 1 | Select the polarity and acquisition mode for an event to add and add the event to the Event Table. |
| 2 | Displays an overview of events for registered data acquisition modes. |
| 3 | Sets the details of the event selected in the Event Table. |

## 3 Sets detailed parameters for events.

Settings differ depending on the data acquisition mode.

**For MRM**

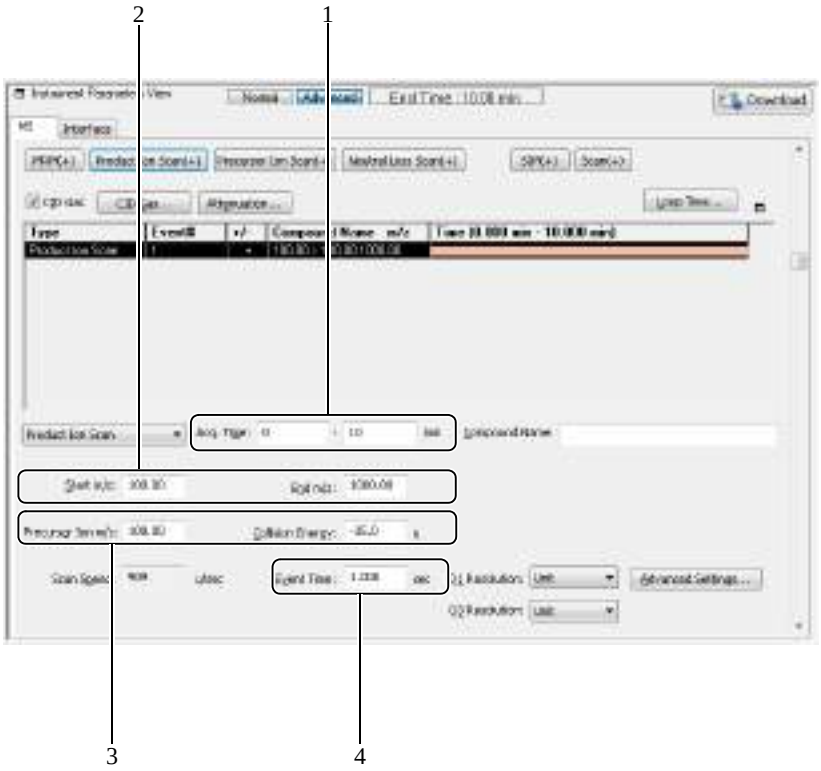
Q1 and Q3 are both parameters for the SIM measurement mode.




| No | Explanation |
|---|---|
| 1 | Sets the measurement start time and end time for the event. |
| 2 | Sets the compound name of the component to measure. Each MRM event sets measurement conditions for one component. |
| 3 | Sets the *m/z* values for precursor ions and product ions obtained by fragmenting precursor ions. Up to 32 channels can be set. Set the target and referenced ion m/z for 1 compound in each channel in the same MS event.The chromatogram in ch1 is used as the target and the chromatogram in ch2 is used as the reference ion by default.<br>Sets the time and collision energy values required to load chromatograms via the specified channel.<br>A method optimization function is available for fine tuning *m/z* values for precursor ions and product ions and automatically searching for product ions.<br>See *"9 Method Optimization" P.285*. |
| 4 | Sets the time required for a single event. When the MS event time is long, the shape of chromatogram will be changed as the sampling rate is long. When the MS event time is short, it will affect the sensitivity and the reproducibly as the sampling rate is short. |

**For Product Ion Scanning**

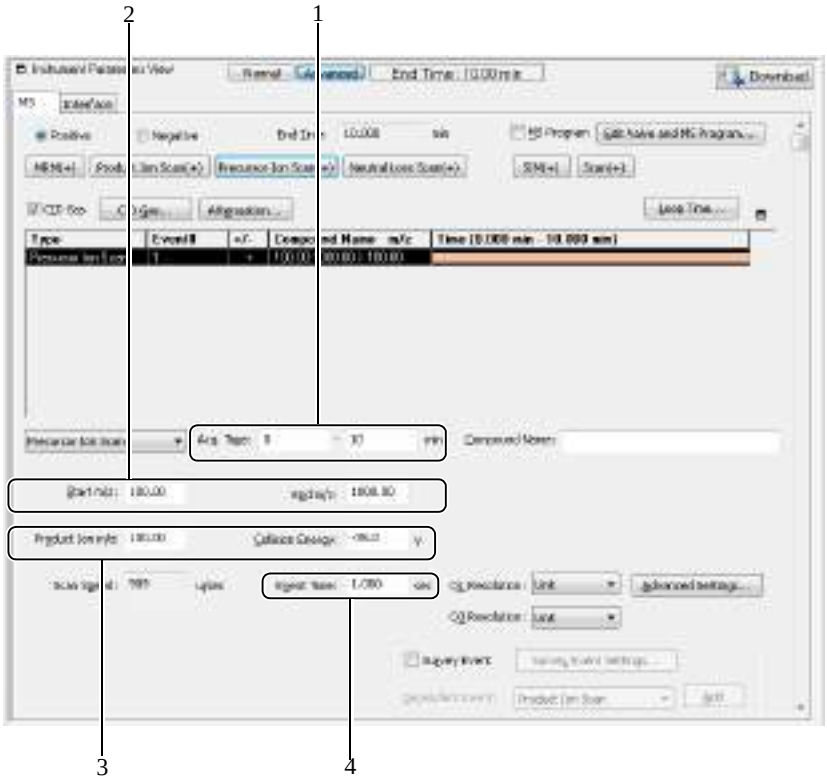
Q1 and Q3 are parameters for SIM and scan measurement modes, respectively.




| No | Explanation |
|---|---|
| 1 | Sets the measurement start time and end time for the event. |
| 2 | Sets the *m/z* range for scan measurements. |
| 3 | Sets the m/z value for the specific precursor ion measured by Q1 and collision energy values to obtaine product ion by fragmenting precursor ions.<br>Fragment ions obtained by fragmenting precursor ions at the *m/z* value set here are measured by Q3. |
| 4 | Sets the time required for a single event. When the MS event time is long, the shape of chromatogram will be changed as the sampling rate is long. When the MS event time is short, it will affect the sensitivity and the reproducibly as the sampling rate is short. |

**For Precursor Ion Scanning**

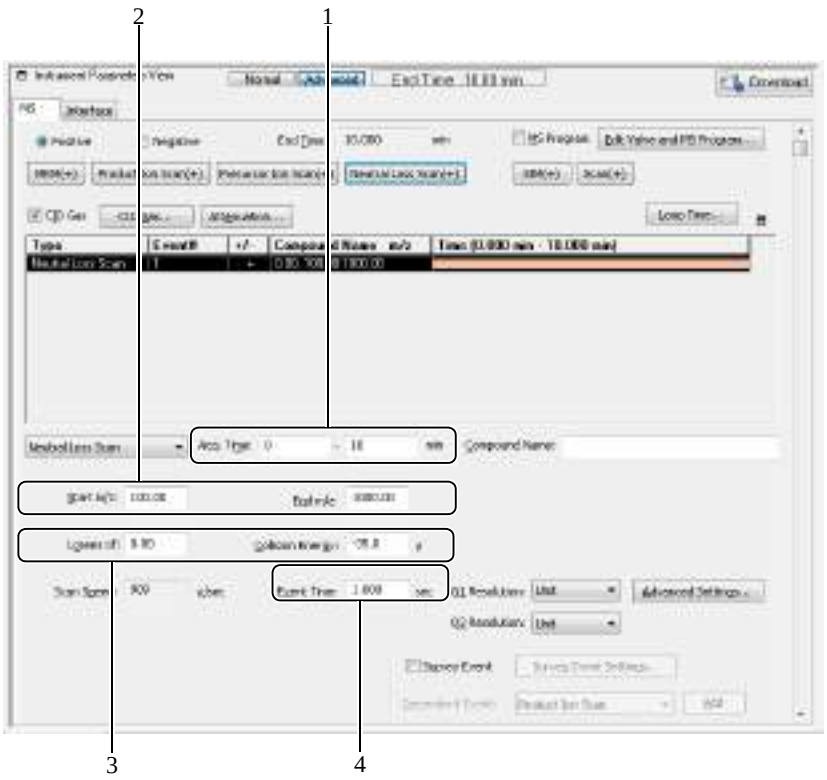
Q1 and Q3 are parameters for scan and SIM measurement modes, respectively.




| No | Explanation |
|---|---|
| 1 | Sets the measurement start time and end time for the event. |
| 2 | Sets the scan range for all precursor ions included in product ions set at [Product Ion m/z]. |
| 3 | Sets the *m/z* value for the specific product ion measured by Q3 and collision energy values to obtaine product ion by fragmenting precursor ions. |
| 4 | Sets the time required for a single event. When the MS event time is long, the shape of chromatogram will be changed as the sampling rate is long. When the MS event time is short, it will affect the sensitivity and the reproducibly as the sampling rate is short. |

**For Neutral Loss Scanning**

Q1 and Q3 are both parameters for the scan measurement mode that keeps the mass difference constant.

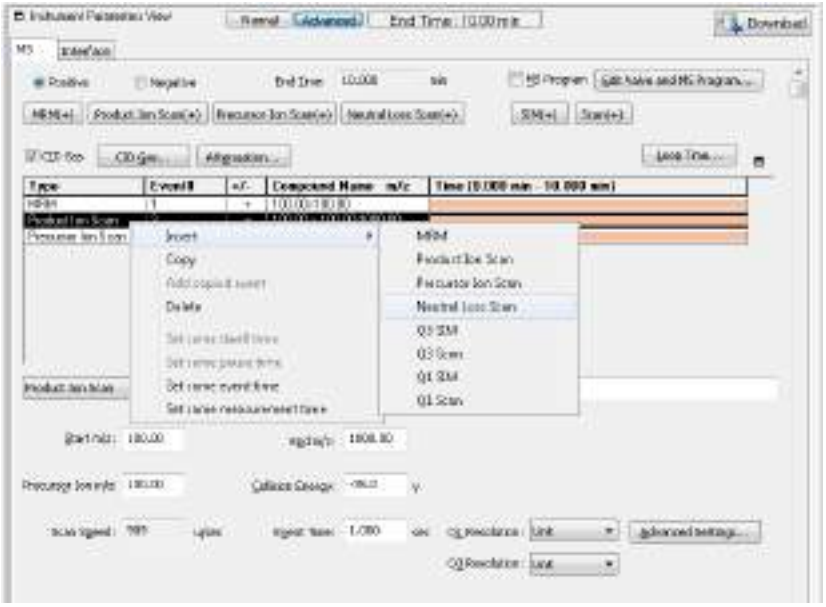



| No | Explanation |
|---|---|
| 1 | Sets the measurement start time and end time for the event. |
| 2 | Sets the *m/z* range of scan measurements. |
| 3 | Sets the neutral loss value and collision energy values to obtaine product ion by fragmenting precursor ions.<br>It scans Q1 in the m/z measurement range, then scans Q3 in the m/z range decreased by this value. |
| 4 | Sets the time required for a single event. When the MS event time is long, the shape of chromatogram will be changed as the sampling rate is long. When the MS event time is short, it will affect the sensitivity and the reproducibly as the sampling rate is short. |

## 4 Repeat steps 2 and 3 to add the event to the Event Table.

## ■ Insert an Event

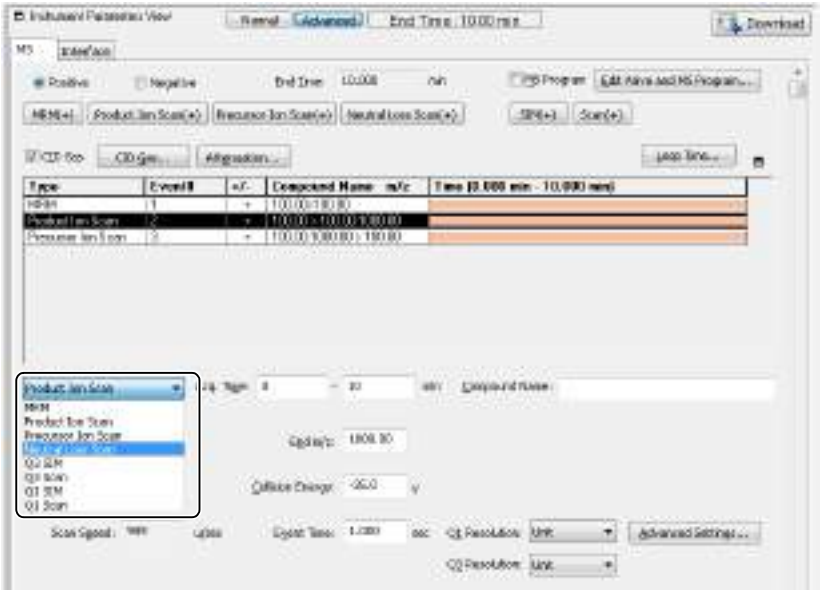
Right-click on the event where the event is to be inserted in the Event Table. Click [Insert] on the displayed menu, and select an appropriate data acquisition mode.



A new event is inserted.

## ■ Change the Data Acquisition Mode

To change the data acquisition mode for an event that is already registered, select an appropriate data acquisition mode from the dropdown list box to the left of [Acq. Time].

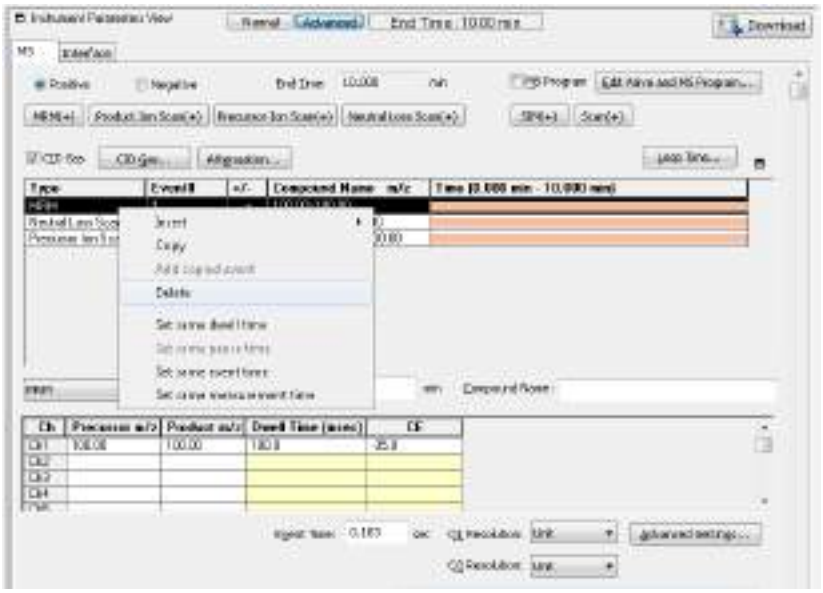


**NOTE**

The polarity cannot be changed for events that are already registered. To change the polarity, register the event again.

## ■ Delete an Event

Right-click on the event to delete in the Event Table, then click [Delete] on the displayed menu.

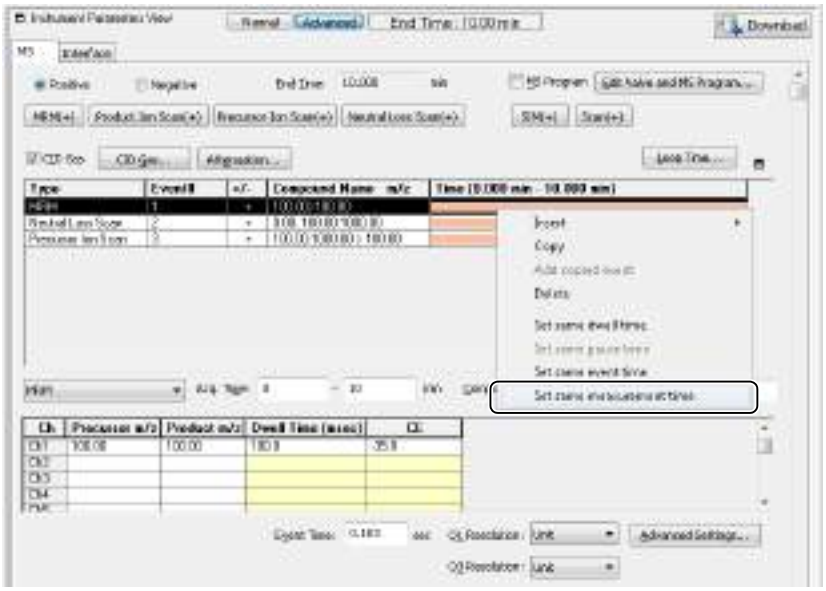


**NOTE**

- Events can also be deleted by selecting the event and pressing the [Delete] key.
- Multiple events cannot be deleted at the same time.

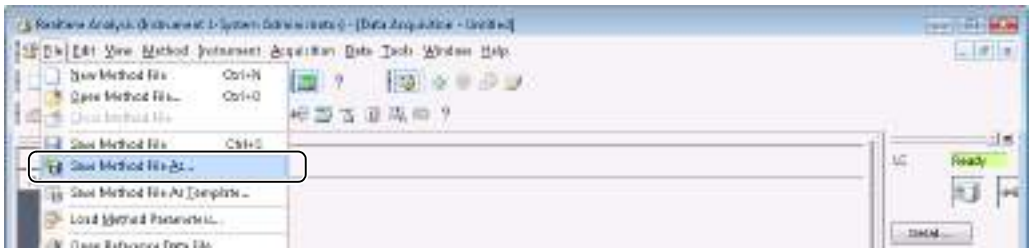
## ■ Set the Same Measurement Time for All Events

Right-click on the events in the Event Table for which the measurement time is entered, then click [Set Same Measurement Time] on the displayed menu.



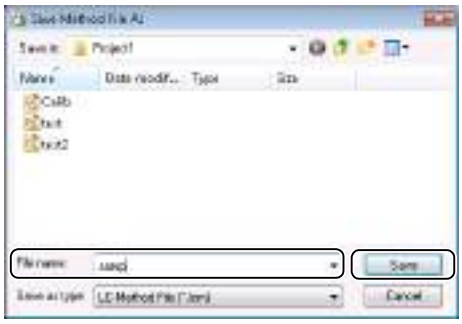
## 2.2.4 Save Data Acquisition Settings in a Method File

**1** **Click [Save Method File As] on the [File] menu.**



The [Save Method File As] window is displayed.

**2** **Enter the file name, and click [Save].**



A method file is created with the specified file name and the new instrument parameters are saved to the file.

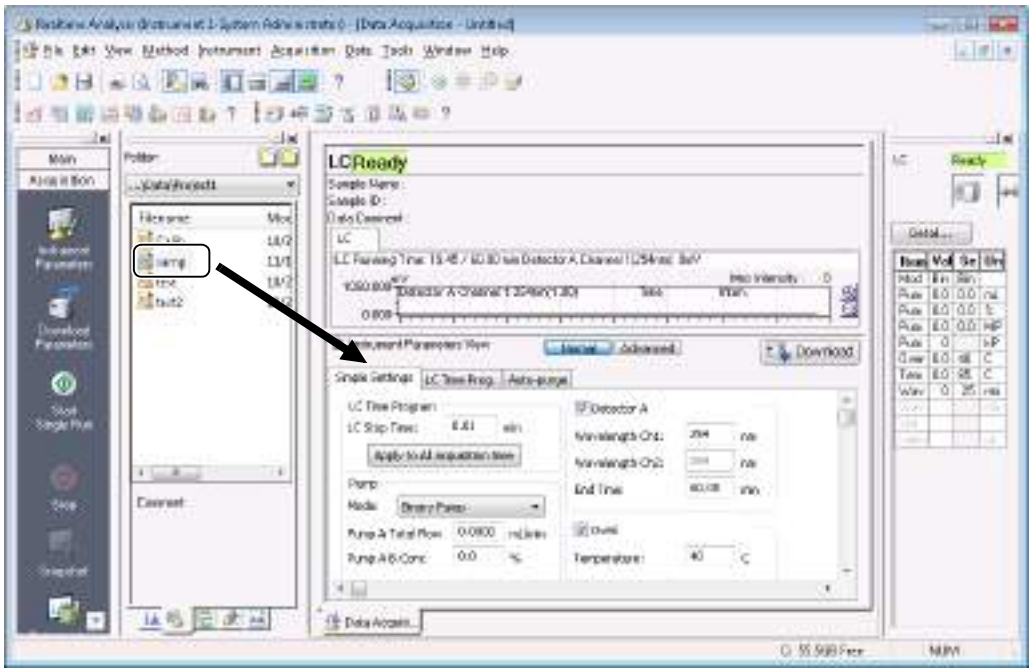
## 2.2.5 Analytical Instrument Startup

This section describes how to transfer (download) instrument parameters to an analytical instrument and the procedure for starting the instrument.

**1** **Drag-and-drop the desired method file onto the [Data Acquisition] window from the [Data Explorer] sub-window.**

**NOTE**

If the [Data Explorer] sub-window is not displayed, click the (Toggle Data Explorer) button on the tool bar.




The content of the method file is displayed in the [Data Acquisition] window.

**2** **Check the instrument parameters, and click Download.**

The instrument parameters are transferred to the analytical instrument.

**3** **Click the (Instrument On/Off) button on the toolbar.**

Pump solvent delivery and oven temperature control are started.

**NOTE**

If the instrument is already activated when the method file is downloaded, operations are started using the downloaded instrument parameters.

**4** **Click (MS Instrument On/Off) on the toolbar.**

DL heater and heat block temperature control are started.

# 2.3 Data Acquisition Preparation

This section describes the procedures to perform before starting data acquisition, such as auto-purging of the pump and autosampler, and verification of column equilibration (baseline check).

## 2.3.1 Monitor the Chromatograms and Instrument Status Curves

This section describes how to monitor chromatograms displayed in [Chromatogram View] and instrument status curves.

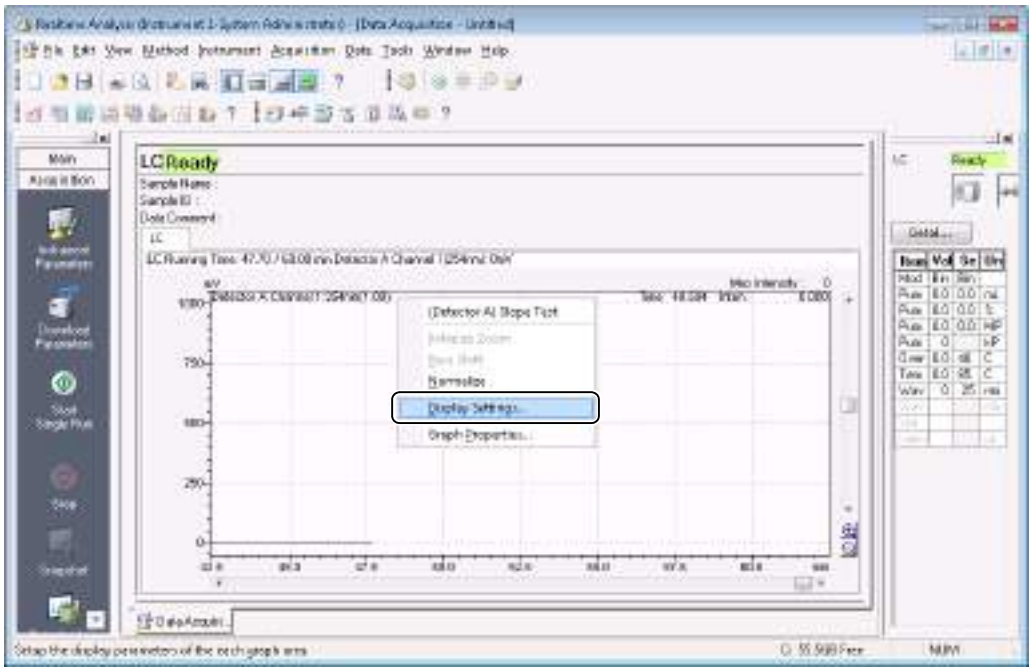


### ■ Chromatogram Display Settings

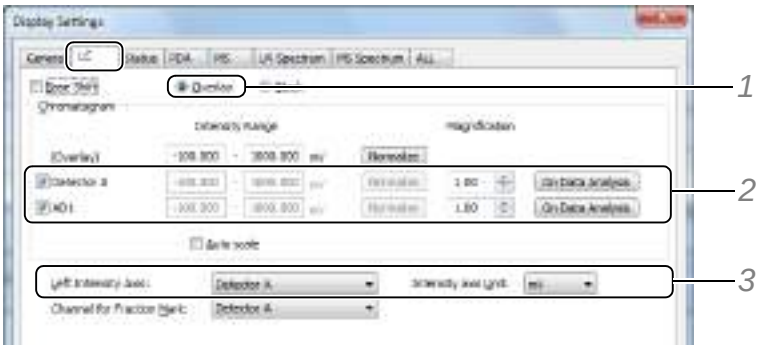
The chromatogram display scale can be changed.

This section describes how to monitor chromatograms on multiple channels.

**1** **Right-click on the graph in [Chromatogram View], and click [Display Settings].**



## 2 Click the [LC] tab and enter the necessary parameters.




1 Click [Overlay] to draw chromatograms overlaid.

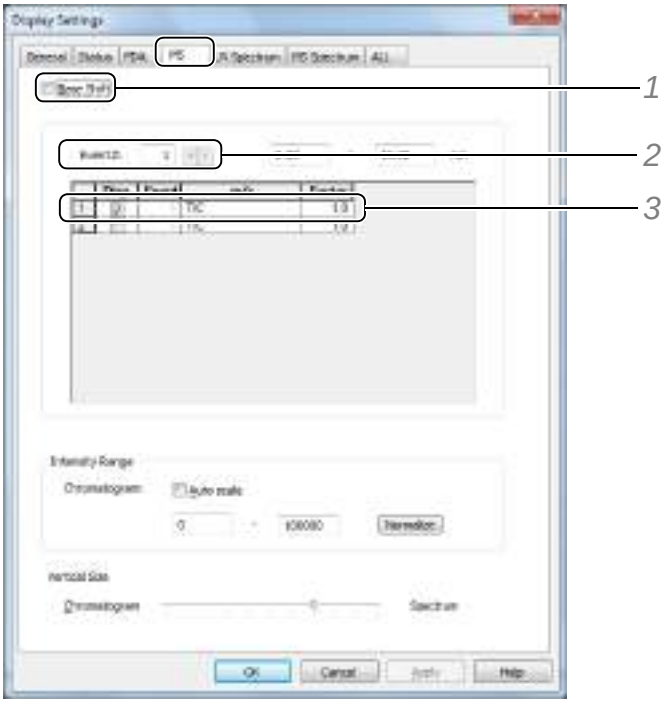
2 Enter the detector intensity range for the Y-axis.
Click [Normalize] so that the intensity range falls within the minimum and maximum values of the currently displayed chromatogram.

3 Select the detector (or channel in Dual Mode) and the display unit for the Y-axis.

**NOTE**

The intensity range of each detector (or channel in Dual Mode) cannot be set in the [Overlay] mode.

## 3 Click the [MS] tab and enter the necessary parameters.

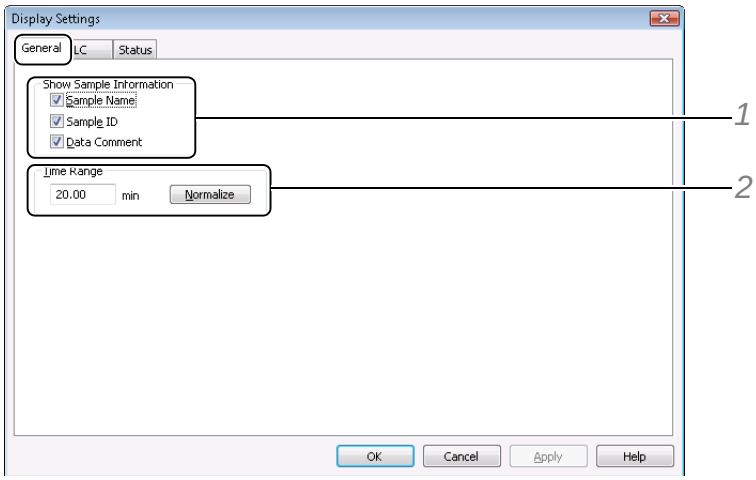



1 Select [Base Shift] to display each MS chromatogram in the Base Shift view.

2 Set the event number of MS chromatograms to display.

3 Enter the *m/z* value of the desired MS chromatogram.
Enter “TIC” to display TIC.
To display an MS chromatogram of an SIM event or MRM event, select the corresponding *m/z* value in the dropdown list box.

## 4 Click the [General] tab, enter the necessary parameters, and click [OK].




*1* Select [Sample Name], [Sample ID] and [Data Comment].
The sample information is displayed in the status display of the [Data Acquisition] window.


*2* Enter the [Time Range] for the X axis display range.
Click [Normalize] to set the display range of the X-axis to either the [LC Stop Time] currently set in the method file or the longest detector time.

## 5 Click the (Save) button on the toolbar.

The time range and intensity range are saved to the method file.

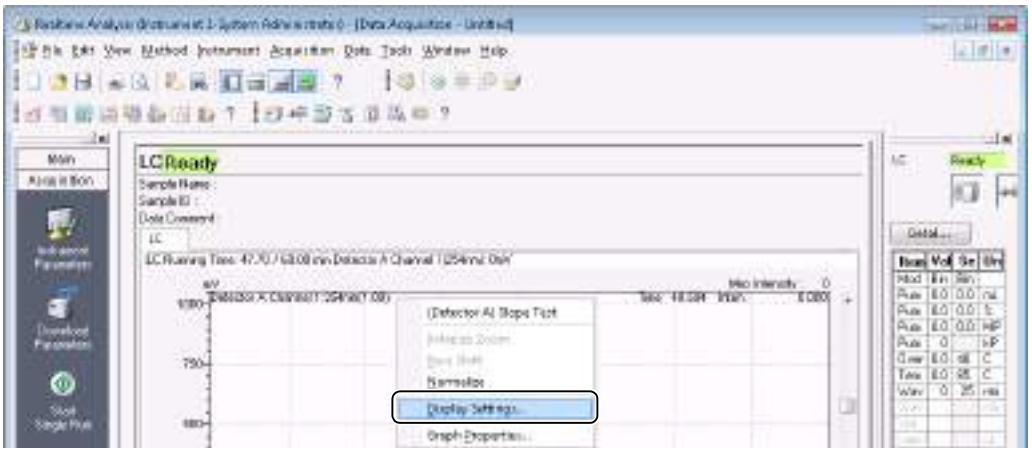
**NOTE**

- Settings other than the time range and intensity range are stored to memory for each user and instrument.
- The [PDA] and [UV Spectrum] tabs are displayed when a PDA detector is used.
- The [MS] and [ALL] tabs are displayed when an MS detector is used.
- Click [Plot] to monitor the multi chromatograms of the PDA detector.
  When the plot is started, the system status changes to [Plot].
  Click [Stop] to stop the plot.
- The reference chromatogram can be drawn overlaying [Chromatogram View].
  Click [Open Reference Data File] in the [File] menu to select and display the reference chromatogram. The reference chromatogram cannot be drawn overlaying MS data.

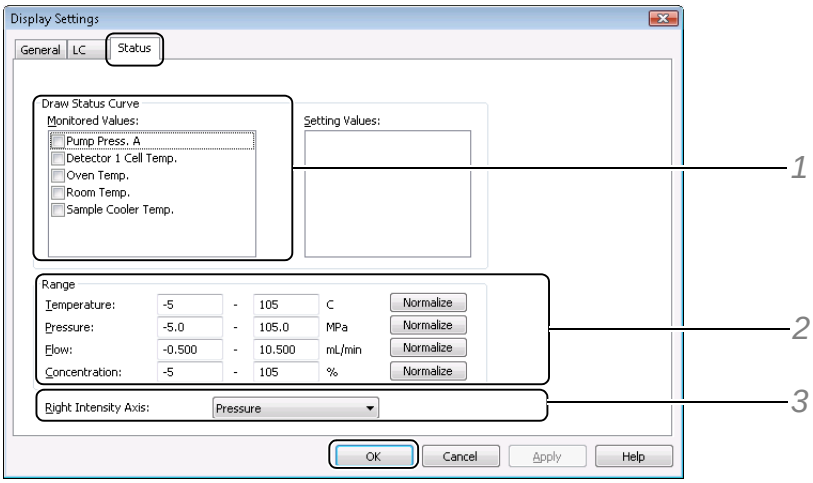
## ■ Display Instrument Status Curves

The instrument status curves that can be displayed on the graph in [Chromatogram View] include [Pump Press.], [Oven Temp.], [Room Temp.], and [Detector Cell Temp.].

**1** **Right-click on the graph in [Chromatogram View], and click [Display Settings].**

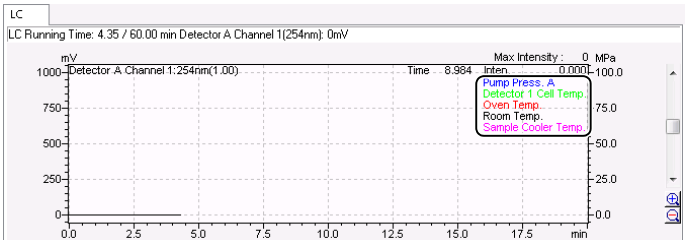



**2** **Click the [Status] tab, enter the necessary parameters, and click [OK].**




*1* Select the desired display items in [Draw Status Curve].
*2* Set the display range for each status item.
*3* Select the type of status to display on the intensity axis on the right of the graph.

The selected status is displayed on the graph.




**NOTE**

- Settings are stored to memory for each user and instrument.
- Status cannot be displayed on MS chromatograms.

## 2.3.2 Auto-Purge the Pump and Autosampler

The mobile phase in the pump and the autosampler syringe rinse solution can be automatically purged.

A function is also provided to deliver solvent at a lower mobile phase flow rate after the autopurge ends until the column oven reaches its preset temperature.

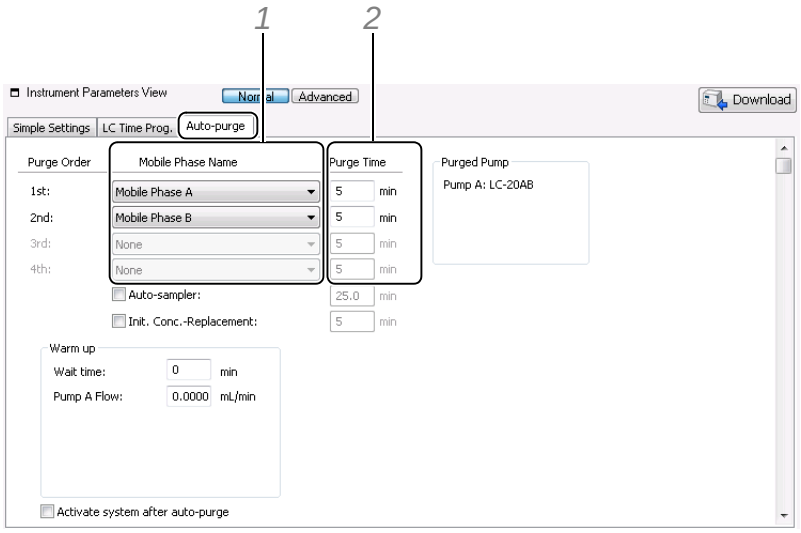
Autopurge is executed in the following order: purging of pump → purging of autosampler → purging at initial concentration conditions (when pump mode is other than Isocratic) → warm up.

**NOTE**

The [Autopurge] tab is displayed when an autosampler is used.

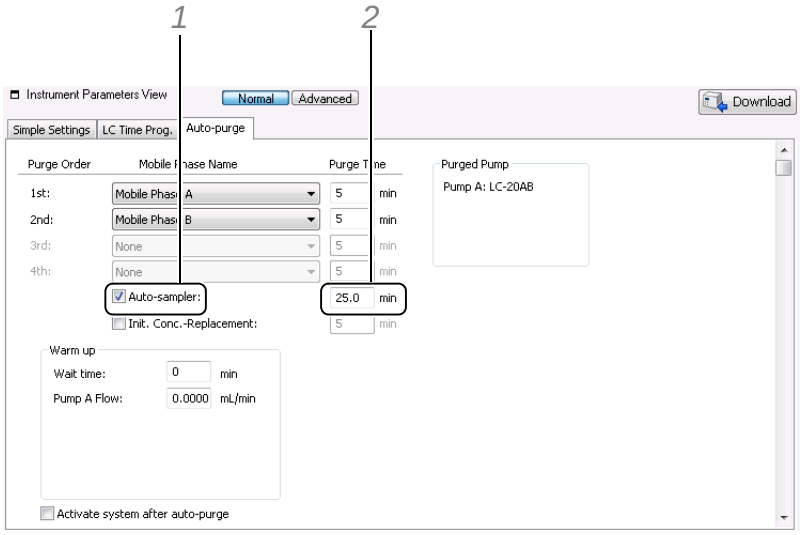


**1 Click the [Autopurge] tab in [Instrument Parameters View], and set the autopurge conditions for the pump.**



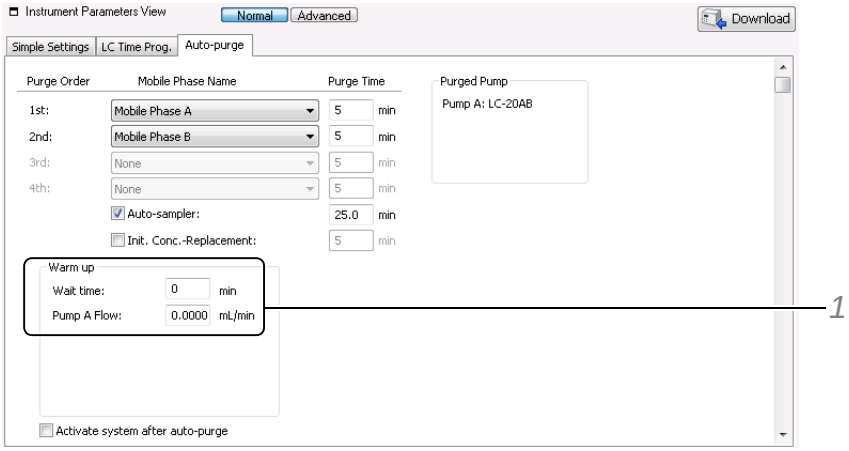

1 Select the lines to be purged from the [Mobile Phase Name] list.
2 Enter a [Purge Time] for each line.

**2 Set the autopurge conditions for the autosampler.**




1 Select [Autosampler] .
2 Enter the [Purge Time].

## 3 Set the [Warm-up] conditions.




1 Enter the [Wait time] and [Flow].

**NOTE**

- [Warm up] is used to deliver solvent at a lower flow rate after purging of the autosampler ends until the oven reaches its preset temperature.
- Enter “0” min at [Wait time] to disable the [Warm up] function.

## 4 Click the (Save) button on the toolbar.

The settings are saved to the method file.

## 5 Click the (Autopurge) button on the toolbar.

Autopurge is started.

**NOTE**

- Click the (Purge autosampler) button on the toolbar. The purge is executed by [Purge Time] set on the [Autosampler] tab.
- After the autopurge ends, column equilibration can be checked using the baseline check function.

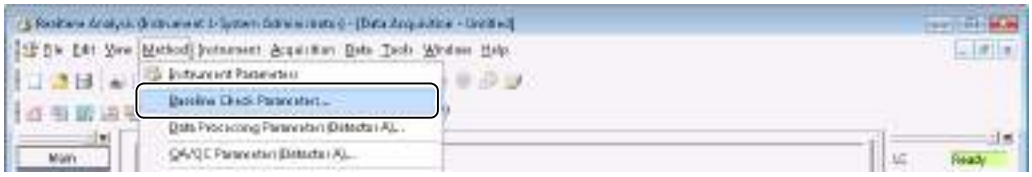
**Reference**

Refer to *"2.3.3 Check the Baseline" P.29* for information on the baseline check procedure.

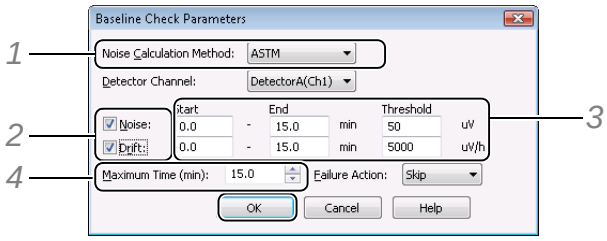
## 2.3.3 Check the Baseline

Use the baseline check function to determine whether the baseline noise and drift values are within the preset time and at or below the threshold for each channel.

**1** **Click [Baseline Check Parameters] from the [Method] menu in the [Data Acquisition] window.**



**2** **Set the baseline check parameters, and click [OK].**




1 Select the noise calculation method.
2 Select [Noise] and [Drift].
3 Enter the time and threshold used for checking [Noise] and [Drift].
4 Enter a [Maximum Time] to performing repeat the evaluation if the checks “fail”.

**NOTE**

Select a [Failure Action] to be taken in the event of a baseline check failure. The [Failure Action] parameter is used when [Baseline Check] is used in the Batch Table.

**3** **Click the (Save) button on the toolbar.**

The settings are saved to the method file.

**4** **Click on the (Baseline Check) button on the toolbar.**

The baseline check is initiated, and the results of the baseline check are displayed after measurement ends.

**NOTE**

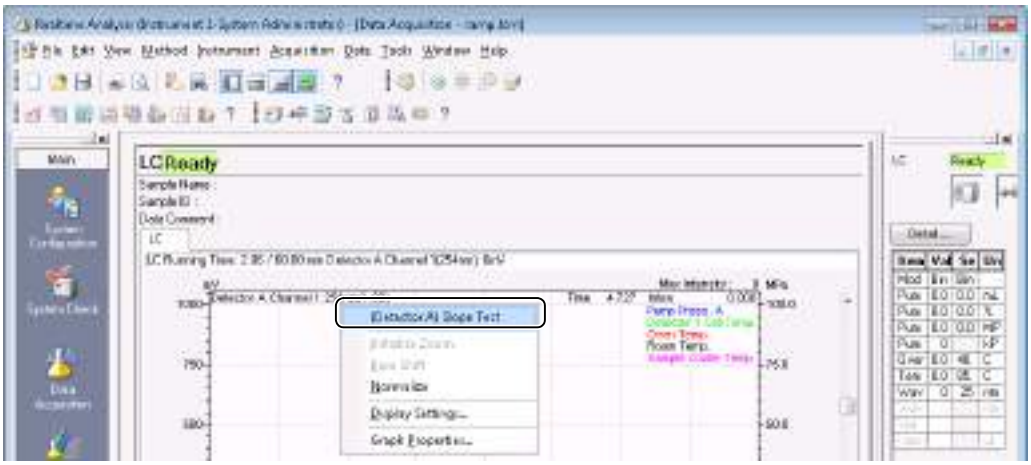
- The results of the baseline check are saved in the C:\LabSolutions\Log\Baseline folder.
- PDA baseline check cannot be performed for a channel set to [Max Plot] in the [Wavelength] column of the [Multi Chrom] tab in the [Data Processing Parameters] sub-window.
- The baseline check cannot be performed for MS detectors.

## 2.3.4 Calculate the Baseline Slope (Slope Test)

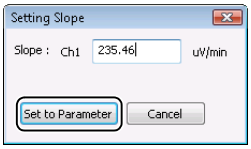
When the Slope Test is performed, the baseline of the chromatogram is measured to automatically calculate the Slope value.

The calculation results of the Slope Test can be set as the Slope value for the peak integration parameters.

**1** **Right-click on the graph in the [Chromatogram View], and click [Slope Test].**




**2** **Click [Set to Parameter] to enter the on-screen value into the data processing parameters.**




The data processing parameter [Slope] value is set.

**NOTE**

- The Slope value is generally rounded up to value that is larger than the calculated value. For example, a Slope value of “1988” is changed to “2000”.
- The Slope Test cannot be performed with MS detectors.

**3** **Click the (Save) button on the toolbar.**

The Slope value is saved to the method file.

**NOTE**

The Slope Test cannot be executed during data acquisition or during PDA plotting.

## 2.3.5 Check the Condition of Consumables (System Check)

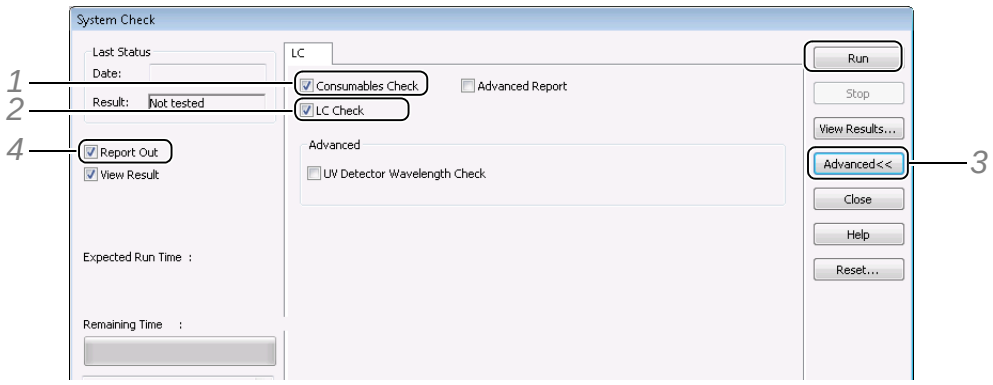
Check the system to verify that it is in good condition before starting data acquisition by checking the use frequency of the instrument consumables (i.e. the system check).

**NOTE**

Users are required to have the [Run System Check] rights to execute the system check.

**1** **Click the (System Check) icon on the [Main] assistant bar.**

**2** **Select the items to check, and click [Run].**

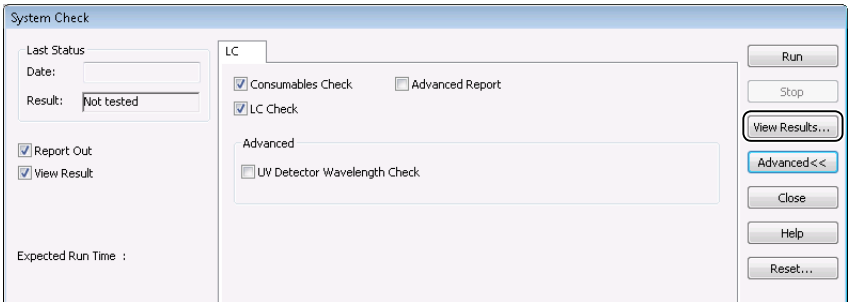



1 Select [Consumables Check].
2 Select [MS Check].
3 Click [Advanced], and select the items to perform the system check on.
4 Select [Report Out] to automatically print the system check results.

**NOTE**

- When using the LC-2010/LC-2010HT, logs recorded on instruments can be displayed in result reports. Up to 50 logs (30 on the CMD) can be displayed.
- When using an LC or photodiode array detector, set the system check method on each of their respective tabs.
- If [Advanced Report] is selected, the system check is executed on all items.
- Click [Advanced] in the [System Check] sub-window, and select [UV Detector Wavelength Check] to simultaneously check the wavelength on the UV detector.

## 3 After the system check ends, click [View Results].




The [System Check Results] sub-window opens.

**NOTE**

- Click [Print] in the [System Check Results] sub-window to print the system check results.
- The system check results are saved to a file named according to the following rule: “SysChk#_YYYYMMDDHHMMSS.lcs” (where, “#” is the system number.)
- To check the results of previous system checks, click [Load] in the [System Check Results] sub-window, and select the desired results.
- Set [System Check] in a Batch Table, to check the use frequency of instrument consumables before starting data acquisition. Refer to *"3.2.3 Batch Table Parameters" P.52* for details.
- Realtime batch can be canceled according to the results of the system check by using the Batch Table action function.
- The system check is based on the consumable criteria of each instrument. Check consumable criteria in the [System Check] sub-window by clicking [System Check] in the [Properties] sub-window of each instrument.
- Click [Reset] to open the [Consumables Reset] sub-window.
  Reset the consumables when they have been replaced.
- Users are required to have the [Edit System Configuration] rights to set system check criteria.

## 2.3.6 Control Toolbar

Change instrument status such as pump solvent delivery on/off, autosampler purge and rinse, oven control on/off, detector zero correction, and MS detector on/off using the [LC Control] toolbar, [PDA Control] toolbar and [MS Control] toolbar.

**NOTE**

The displayed buttons vary depending on the system configuration of the instrument.



### [LC Control] toolbar

| Button | Name | Explanation |
|---|---|---|
| | Instrument On/Off | Turns the ACTIVATE feature of the SCL-10Avp/SCL-10Asp system controller on/off.<br>This button controls the pump and column oven for the CBM-20A/20Alite. |
| | Controller LCD On/Off | Turns the LCD of the SCL-10Avp/SCL-10Asp system controller on/off. |
| | Controller Lock/Unlock | Locks or unlocks keypad control of the SCL-10Avp/SCL-10Asp system controller. Only software control is permitted when keypad control is locked. This button is used to prevent operational errors. |
| | Pump On/Off | Turns the solvent delivery pump on/off. |
| | Purge autosampler | Executes an autosampler purge according to the [Purge Time] set on the [Autosampler] tab in [Instrument Parameters View]. |
| | Rinse autosampler | Rinses the autosampler and sampling needle. |
| | Oven On/Off | Turns the column heater oven on/off. |
| | Zero Detector A | Returns the signal intensity of detector A to zero. |

### [PDA Control] toolbar

| Button | Name | Explanation |
|---|---|---|
| | PDA Detector Lamp On/Off | Turns the PDA detector lamp on/off. |
| | Zero PDA Detector | Returns the signal intensity of the PDA detector to zero. |

### [MS Control] toolbar

| Button | Name | Explanation |
|---|---|---|
|  | MS Instrument On/Off | Turn on/off the heater and gas in 1 operation. |
|  | Open/Close Drying Gas | Turns the drying gas on/off.<br>**NOTE**<br>This item is displayed for an ESI, DUIS, APCI or Micro-ESI interface. |
|  | Open/Close Nebulizing Gas | Turns the nebulizer gas on/off.<br>**NOTE**<br>This item is displayed for an ESI, DUIS, APCI or Micro-ESI interface. |
|  | Open/Close Heating Gas | Turns the heating gas on/off.<br>**NOTE**<br>Displayed for LCMS-8045/8050/8060 systems with an ESI, DUIS or Micro-ESI interface. |
|  | Interface Heater On/Off | Turns the interface heater on/off.<br>**NOTE**<br>Displayed for LCMS-8045/8050/8060 systems with an ESI, DUIS or Micro-ESI interface. |
|  | DL On/Off | Turns the heater of the DL on/off. |
|  | Interface Heater On/Off | Turns the APCI heater on/off.<br>**NOTE**<br>This item is displayed for an APCI interface. |
|  | Heat Block On/Off | Turns the heater of the heat block on/off. |
|  | IG On/Off | Turns the IG (ion gage) on/off. |
|  | MS Detector On/Off | Turns the MS detector on/off. |

**NOTE**

If the toolbar is hidden, use the right-click popup menu on the menu bar, and select the desired toolbar from the displayed menu.

## 2.3.7 Instrument Monitor

[Instrument Monitor] displays the instrument status and parameter settings. The instrument settings can be changed without changing the instrument parameters in the method file by entering a value in the [Setting] cell.

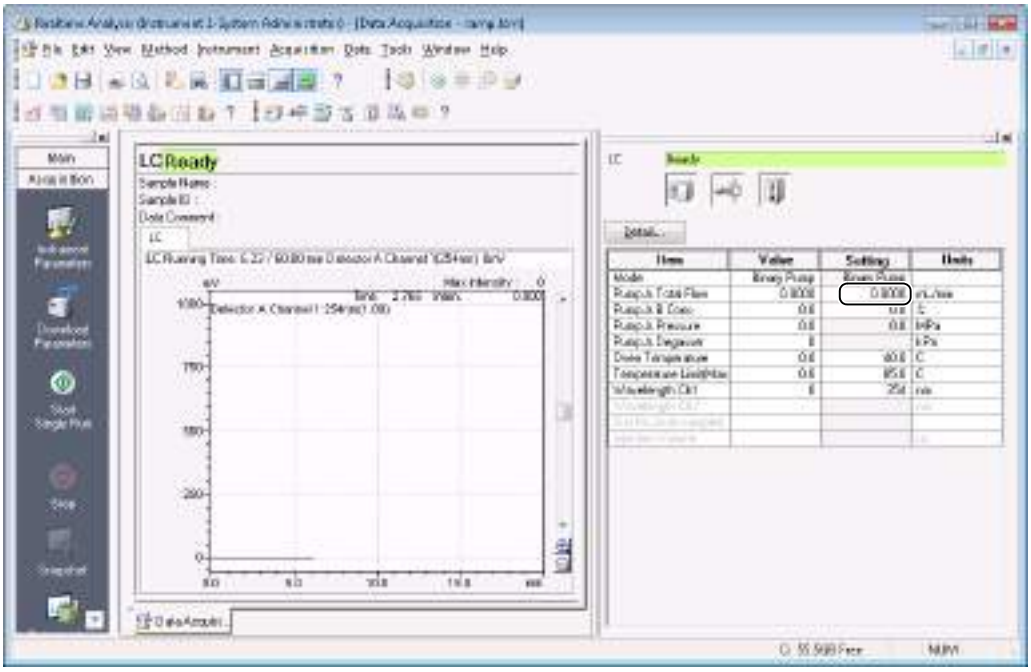
This section describes the procedure for changing the pump flow rate [PumpA. Flow].

**NOTE**

If the [Instrument Monitor] is not displayed, click the (Toggle Instrument Monitor) button on the toolbar.



**1** **Click the [Pump A Total Flow] cell in the [Setting] column, and enter the new pump flow rate.**




**2** **Press the [Enter] key.**

The flow rate is changed.

**NOTE**

- Change the displayed status items in [Instrument Monitor] in the [Table Style] sub-window. Right-click on [Instrument Monitor], and select [Table Style] from the displayed menu.
- If the value in the [Setting] column is changed in [Instrument Monitor], it is not saved to method file.
  Details of changes under analysis made are recorded in the operation log, and can be checked in the [Logs] sub-window. This sub-window is opened by clicking [Acquisition Log] on the [View] menu in the [Data Analysis] / [PDA Data Analysis] / [MS Data Analysis] window

# 2.4 Plot

Verify that the MS detector baseline is stable before acquiring data.

1 **Check [Instrument Parameter View] and click Download.**

2 **Click [MS Instrument On/Off] on the [MS Control] toolbar.**

The nebulizer gas is turned on, and heating of the DL and other operations are started.

3 **When the temperature of the DL and heat block reaches the set value on [Instrument Monitor], click the [Plot] icon in the chromatogram view.**

Verify that the MS detector baseline is stable.

# 2.5 Single Run

There are two ways of acquiring data, by single run (only one data acquisition), or by realtime batch (sequential analysis of multiple samples).

This section describes the procedure for a single run.

**NOTE**

Verify that [Ready] is displayed on the status display.

**Reference**

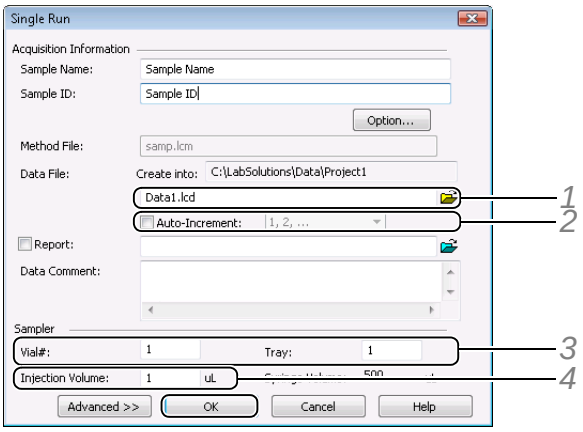
Refer to *"3 Realtime Batch" P.43* for information on sequential analysis of multiple samples.

## 2.5.1 Execute Single Run

Execute single run from the [Data Acquisition] window.

1 **Click the (Start Single Run) icon on the [Acquisition] assistant bar.**

## 2 Set the acquisition conditions, and click [OK].




1 Enter the data file name.

2 Select [Auto-increment], and the number type.
The data file name is automatically appended with an incremental number.
Example: “TEST-001.lcd”

**NOTE**
When [Auto-increment] is selected, the file is not overwritten even if the file name was previously used.

3 Enter the position of the sample for [Vial#] and [Tray].

**NOTE**
Enter “-1” to acquire data without injecting samples from the autosampler.

4 Enter the sample injection volume.

Single run is started.
During data acquisition, the [LabSolutions Service] icon in the Systray on the Taskbar flashes green.


Data acquisition ends when the data acquisition time in the method file has elapsed.

**NOTE**
Do not turn the PC off while the [LabSolutions Service] icon is flashing.

## 2.5.2 Change the End Time During Data Acquisition

The data acquisition time can be changed during data acquisition.

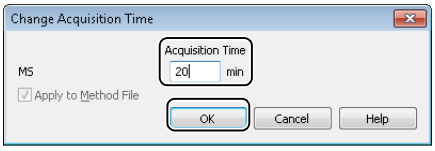
This section describes the procedure for changing the data acquisition time.

**NOTE**

- During data acquisition, [LC Stop Time] on the [Simple Settings] tab in [Method View] cannot be changed.
- If the acquisition time is changed using [Change Acquisition Time], a record is created in the operation log.

**1** **Click [Change Acquisition Time] on the [Acquisition] menu.**


**2** **Enter an [Acquisition Time], and click [OK].**




**NOTE**

- If multiple detectors are used, click [All Times Change] to changes the data acquisition time to the longest detector acquisition time.
- If [Change to Minimum Value] is selected, click [All Times Change] to change the data acquisition time to the shortest detector acquisition time.
- Click [Apply to Method File] to apply the new acquisition time to the method file and use it for all subsequent data acquisitions. However, the MS detector cannot be changed if [Apply to Method File] is selected.
- The MS detector data acquisition time can be lengthened but not shortened.
- You can not change the value as an analysis time that already passed.

## 2.5.3 Stop Single Run

Single run can be stopped in the midway to end acquisition earlier than the preset end time.

**1** **Click the (Stop) icon on the [Acquisition] assistant bar.**

Data acquisition is stopped, and a data file is created for the data so far.

# 2.6 Check Analysis Results During Data Acquisition (Snapshot)

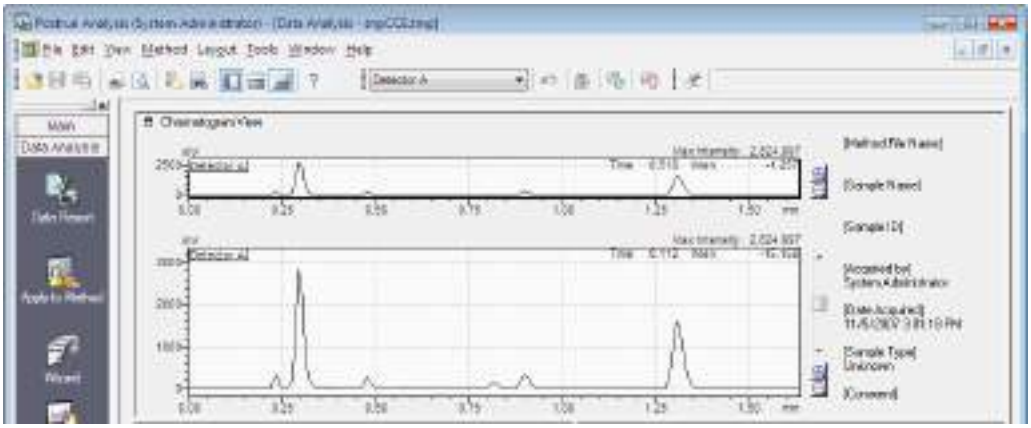
Execute snapshot during data acquisition to display and process the data obtained since acquisition was started.

This section describes the procedure for executing a snapshot during data acquisition.



1 **Click the (Snapshot) icon on the [Acquisition] assistant bar.**

The data obtained so far is displayed in the [Data Analysis] window.



## 2.6.1 Update Snapshots

Use snapshot update to load cumulative acquired data from a continuing data acquisition after snapshot has been executed.

1 **Click the (Update for Snapshot) button on the toolbar in the [Data Analysis] window.**

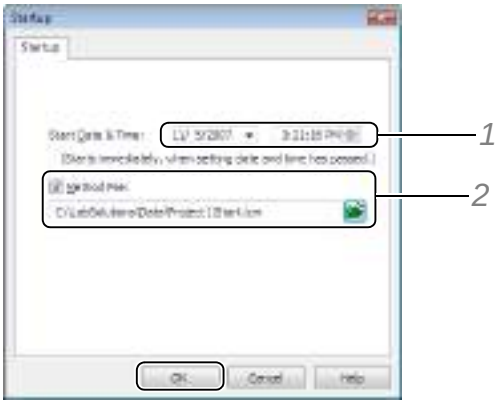
The snapshot is updated to display the latest chromatogram.

# 2.7 Automatic Instrument Startup

Use (Startup) to automatically start the instrument at a specified date and time.

**1** **Click the (Startup) button on the toolbar.**

**2** **Enter the date and time to start the instrument, and click [OK].**




1 Set the date and time to start the instrument.
2 Select [Method File], and enter the method file name. The method file can also be selected by clicking .

**NOTE**

When the method file is not specified, the analytical instrument is started up by the parameters already downloaded to the instrument (i.e. parameters used in the previous data acquisition) when a startup is performed.

The instrument starts up at the specified date and time.

**NOTE**

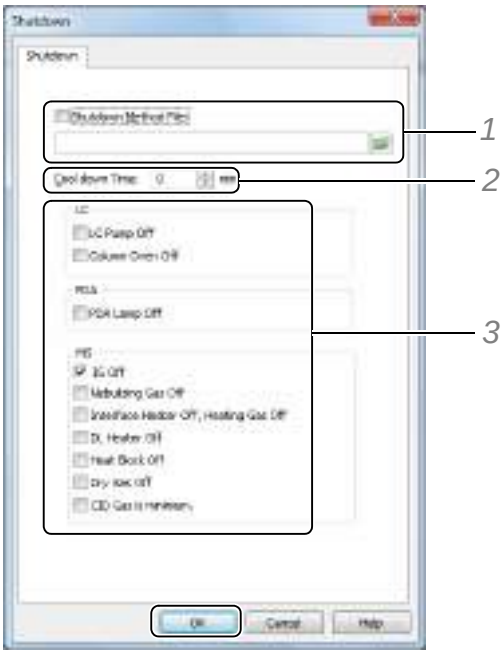
- If startup is executed in a batch file(s) registered to the batch queue, the startup begins after processing of the previously registered batch file(s) ends.
  For details on the procedure for changing the execution order of batch files registered to the batch queue, refer to *"3.5 Data Acquisition Using the Batch Queue Function" P.66*.
- Startup can also be set in realtime batch.
  For details, refer to *"3.4.2 Start Data Acquisition at a Specified Date and Time (Startup)" P.59*.

# 2.8 Automatic Instrument Shutdown

Use [Shutdown] to automatically shut down the instrument after data acquisition ends.

**1** **Click the (Shutdown) button on the toolbar.**

**2** **Set Cool down Time to shut down the instruments, and click [OK].**




*1* Select [Shutdown Method File], and enter the method file name. The method file can also be selected by clicking .

**NOTE**

When a method file is not specified, the analytical instruments are shut down by the parameters already downloaded to the instruments when a shutdown is performed.

*2* Enter the time that the instrument is operated by the instrument parameters of the specified method file.

*3* Select relevant checkboxes for the gas, heater, or other units to switch off when shutting down the instrument.

The analytical instruments shut down when the [Cool down Time] elapses.

**NOTE**

- When [Real Time Analysis Window Close] is selected, the [Realtime Analysis] program is exited after the analytical instruments are shut down.
- If shutdown is executed in a batch file(s) registered to the batch queue, the shutdown begins after processing of the registered batch file(s) ends.
  For details on the procedure for changing the execution order of batch files registered to the batch queue, refer to *"3.5 Data Acquisition Using the Batch Queue Function" P.66*.
- Shutdown can also be set in realtime batch.
  For details, refer to *"3.4.3 Shutdown Analytical Instruments After Data Acquisition (Shutdown)" P.60*.

# 3 Realtime Batch

Realtime batch is sequential data acquisition of multiple samples. Execution of realtime batch starts with the preparation of a Batch Table.

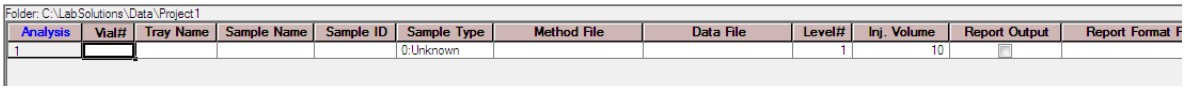
This chapter describes the procedures for automating data acquisition.

- Making Batch Tables
- Baseline check to verify the stability of the baseline
- [Startup] to begin realtime batch analysis at a specified date and time
- [Shutdown] to shutdown the instrument after realtime batch ends



## 3.1 Display Batch Tables

Click the  (Realtime Batch) icon on the [Main] assistant bar in the [Realtime Analysis] program to display the Batch Table.




## 3.2 Create Batch Tables

Enter the sample information, vial #, method file name, and data file name in a Batch Table to sequentially acquire data from multiple samples.

This section describes how to create a Batch Table

### 3.2.1 Batch Table Wizard

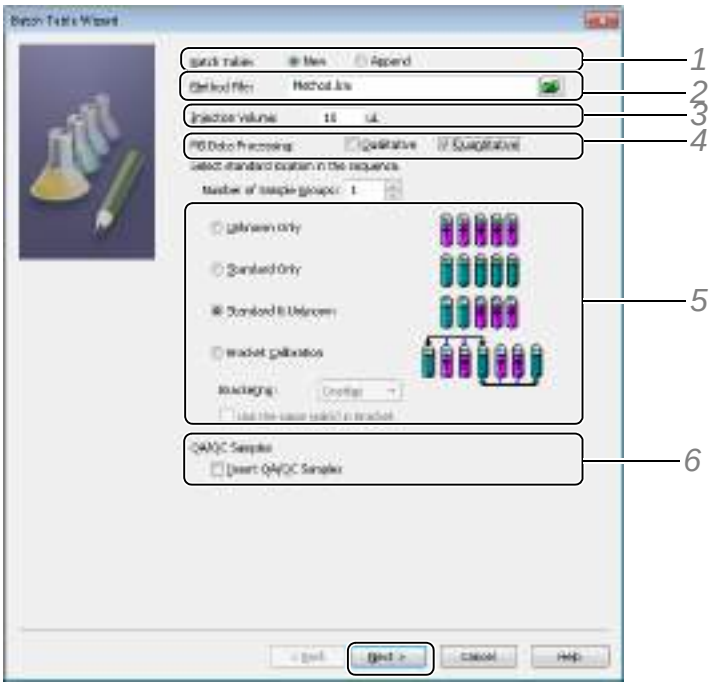
Batch Tables can be made easily by using the Batch Table Wizard.

**NOTE**

Some features of the Batch Tables cannot be set with the Batch Table Wizard. It is necessary to directly edit the Batch Table to set these functions.

1 **Click the  (Wizard) icon on the [Realtime Batch] assistant bar.**

## 2 Enter the parameters, and click [Next].




1 Click [New] at [Batch Table] to create a new Batch Table file.
Click [Add] to add a row to the currently displayed Batch Table.

2 Enter the [Method File].

3 Enter the [Injection Volume].

4 Select [Qualitative] or [Quantitative] at [MS Data Processing].

5 Enter the data acquisition pattern for the standard samples and unknown samples.

Enter a number for [Number of Sample Groups] to indicate the number of times the data acquisition pattern will be repeated.

Select [Bracket Calibration] to select the type of bracket quantitation.

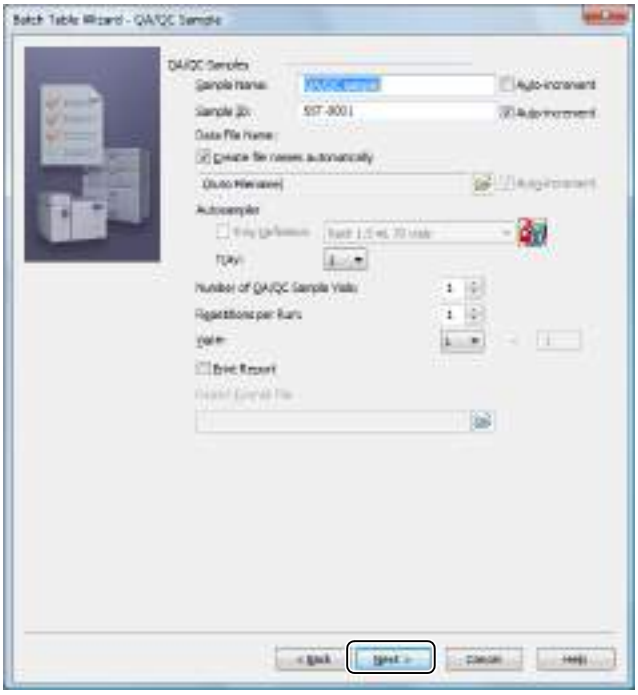
**Reference**

For details, see *"3.4.6 Bracket Quantitation" P.64*.

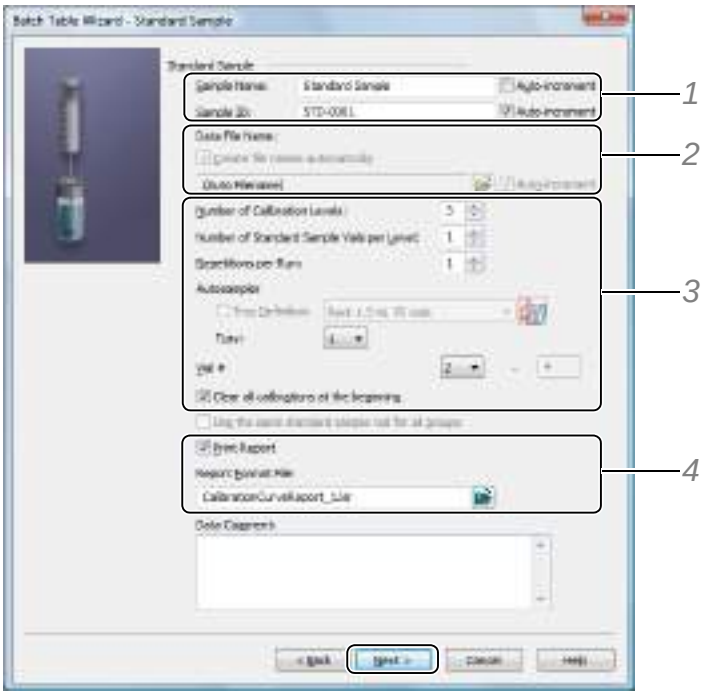
6 Select [Insert QA/QC Samples] to insert a QA/QC sample.

If [Insert QA/QC Samples] is selected, the [Batch Table Wizard - QA/QC Sample] sub-window is displayed. If [Insert QA/QC Samples] is deselected, proceed to Step 4.

**3** **Enter the QA/QC sample information, then click [Next].**



## 4 Enter the standard sample information, and click [Next].




1 Enter [Sample Name] and [Sample ID] for the standard sample.

If [Auto-increment] is selected, the [Sample Name] and [Sample ID] are automatically appended with an incremental number.

2 Enter a [Data File Name].

Select [Create file names automatically] to automatically generate a data file name.

**Reference**

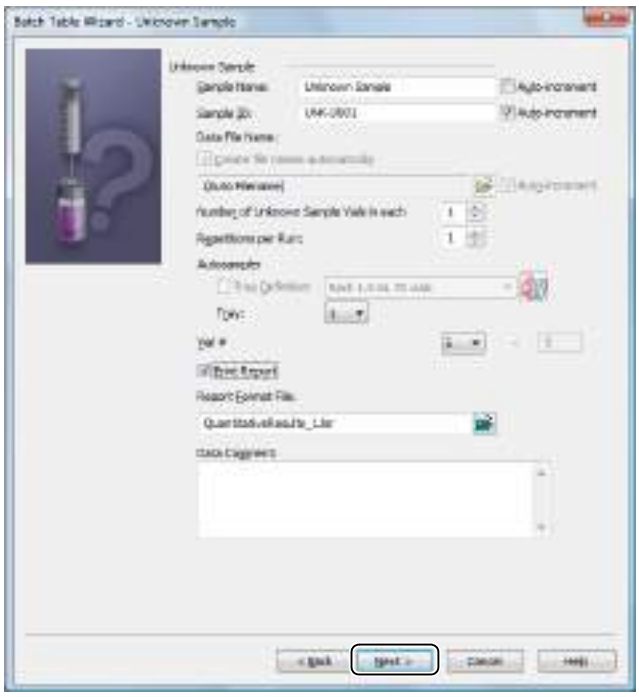
For details, see *"Set the Data File Name" P.75*.

3 Set the [Number of Calibration Levels], [Repetitions per Run] and select [Clear all calibrations at the beginning] to initialize the calibration curve.

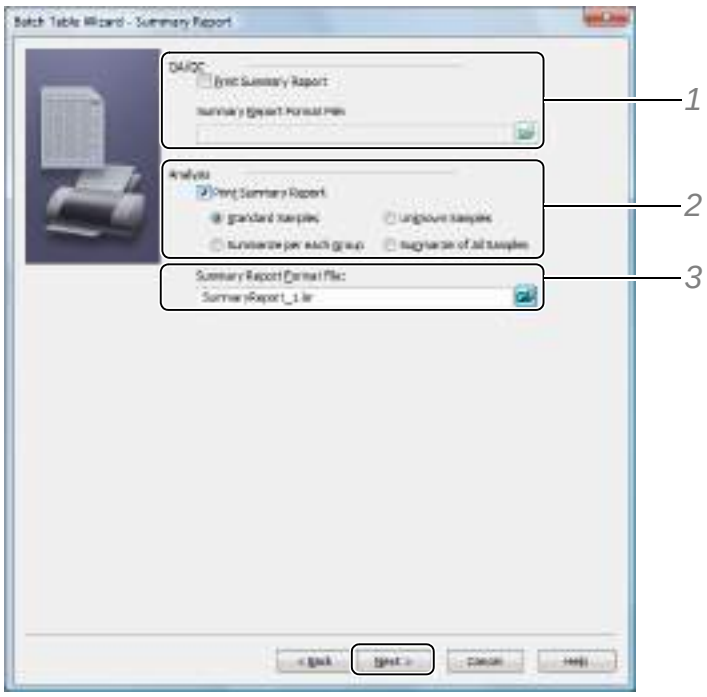
The final vial No. of the standard sample you have set is displayed at [Vial#] in the Batch Table.

4 Select [Print Report] and set [Report Format File] to create reports.

**5** **Enter the unknown sample information, as with the standard sample, and click [Next].**



**6** **Set the summary report output parameters, and click [Next].**




*1* Select [Print Summary Report] for [QA/QC], and select a [Summary Report Format File].

**NOTE**

[QA/QC] is not displayed if [Insert QA/QC Samples] is deselected in the [Batch Table Wizard] sub-window.

*2* Select [Print Summary Report] for [Analysis], and select the type of sample summary that will be reported.

*3* Select the [Summary Report Format File].

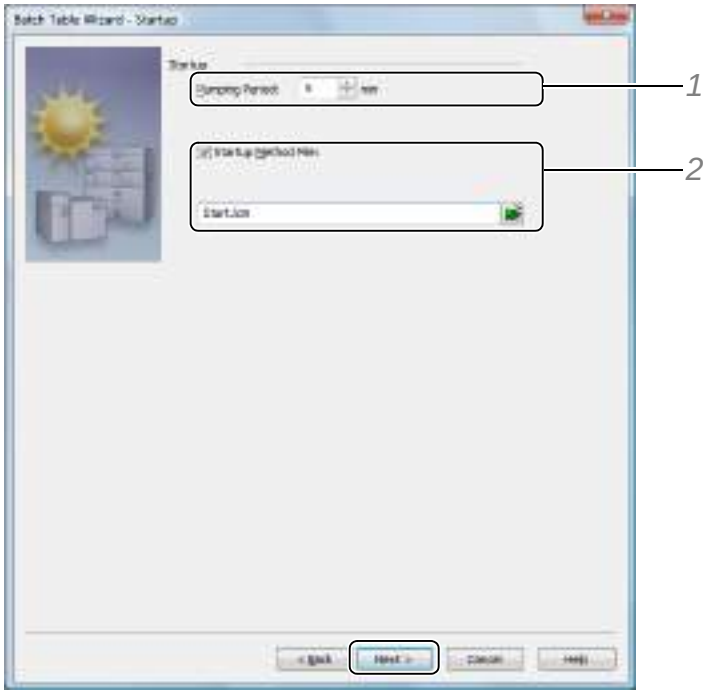
## 7 Select the items to be executed, and click [Next].

If [Startup] or [Shutdown] are selected, a setting sub-windows for each item is displayed. (Steps 8 or 9)
If all of these items are deselected, proceed to Step 10.

## 8 Select the startup settings, and click [Next].

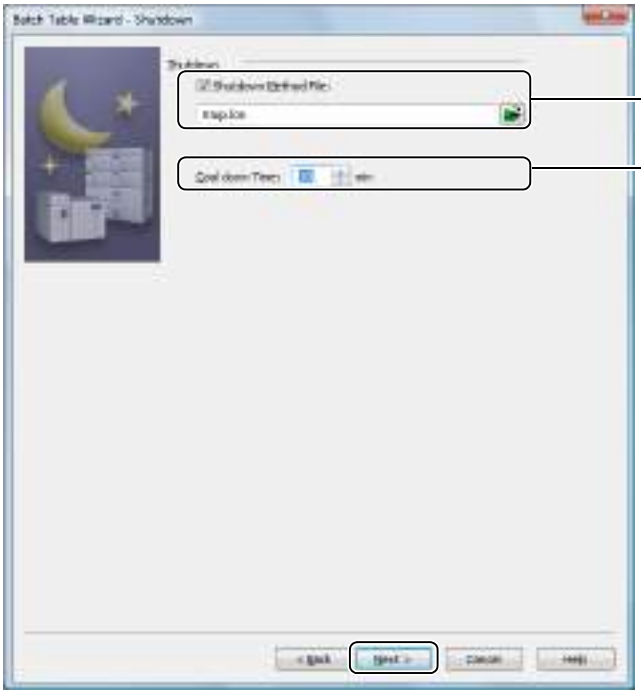
**NOTE**

The startup start date and time cannot be set in the Batch Table Wizard. Refer to *"3.4.2 Start Data Acquisition at a Specified Date and Time (Startup)" P.59* to enter a specified date and time.



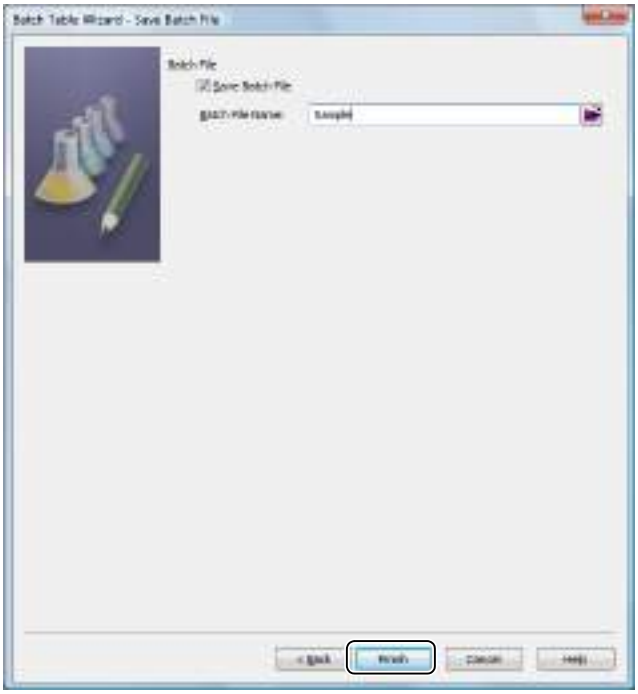

1 Enter an instrument startup time at [Pumping Period].
2 Select [Startup Method File], and enter the method file.

## 9 Select the shutdown settings, and click [Next].




1 Select [Shutdown Method File], and enter the method file.
2 Enter an instrument shutdown time at [Cool down Time].

## 10 Enter a batch file name, and click [Finish].



This completes Batch Table setup using the Batch Table Wizard. The batch file is created using the specified file name. This Batch Table is displayed in the Batch Table sub-window. Check the contents of the Batch Table.

## 3.2.2 Edit Batch Tables

This section describes 2 functions, [Fill Series] and [Fill Down], that are often used for direct Batch Table editing.

### ■ Append Table Settings with an Incremental Number

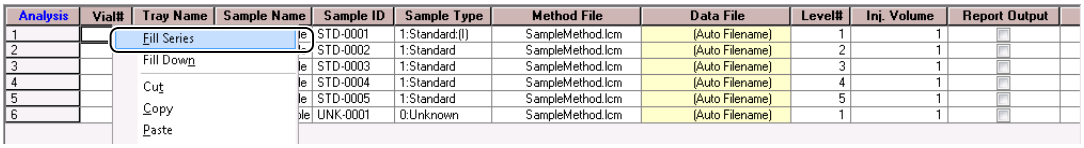
The [Vial#], [Sample Name], [Sample ID], and [Data File] entries in the Batch Table are appended with an incremental number.

This section describes how to add an incremental extension to the [Vial#].

**1** **Click the [Vial#] for the top row.**

| Analysis | Vial# | Tray Name | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# | Inj. Volume | Report Output |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | 1 | Standard Sample | STD-0001 | 1:Standard:(I) | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |
| 2 | | 1 | Standard Sample | STD-0002 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 2 | 1 | |
| 3 | | 1 | Standard Sample | STD-0003 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 3 | 1 | |
| 4 | | 1 | Standard Sample | STD-0004 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 4 | 1 | |
| 5 | | 1 | Standard Sample | STD-0005 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 5 | 1 | |
| 6 | | 1 | Unknown Sample | UNK-0001 | 0:Unknown | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |

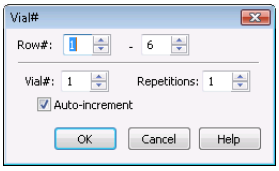
**2** **Right-click the top [Vial#] cell, and click [Fill Series] from the displayed menu.**




**NOTE**

If [Vial#] is blank, the [Vial#] sub-window opens. If a value is entered in the [Vial#] cell that value is used incrementally fill the [Vial#] cells in the rest of the table.

**3** **If the [Vial#] sub-window is displayed, enter the [Row#], [Vial#], [Repetitions], and select [Auto-increment], then click [OK].**



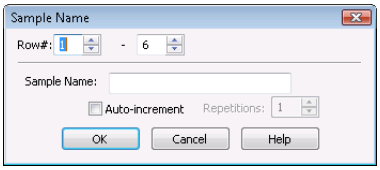

The [Vial#] column is incrementally filled.

| Analysis | Vial# | Tray Name | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# | Inj. Volume | Report Output |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | | Standard Sample | STD-0001 | 1:Standard:(I) | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |
| 2 | 2 | | Standard Sample | STD-0002 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 2 | 1 | |
| 3 | 3 | | Standard Sample | STD-0003 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 3 | 1 | |
| 4 | 4 | | Standard Sample | STD-0004 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 4 | 1 | |
| 5 | 5 | | Standard Sample | STD-0005 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 5 | 1 | |
| 6 | 6 | | Unknown Sample | UNK-0001 | 0:Unknown | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |

### [Fill Series]

[Fill Series] functions according to how the cell is selected and the value entered in the cell.

- If the end of the character string is not a number (ex: “standard sample”)
  A 3-digit number is appended starting with the row following the selected cell.
  “standard sample”, “standard sample 001", “standard sample 002", and so forth.
- If the end of the character string is a number (ex: “STD01”)
  The cells are filled with STD01, STD02, STD03 and so forth.
- If only 1 cell is selected (ex: “ABC”)
  The cells following the selected cell become ABC001, ABC002, ABC003 and so forth.
- If multiple cells are selected (ex: “STD1”, “AAA” and “STD5” are selected in this order)
  The selected cells are changed to STD1, STD2, and STD3.
- If a blank cell is selected (ex: a cell in the [Sample Name] column)
  The [Sample Name] sub-window opens. Enter the sample name parameters, and click [OK].

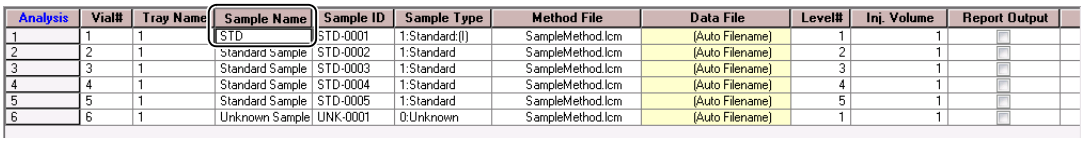



## ■ Copy Settings

The individual columns of the Batch Table can be copied.

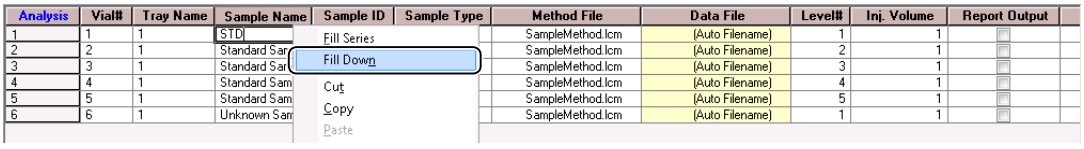
This section describes how to copy and fill the [Sample Name] column.

**1** **Enter a [Sample Name] in the top row.**

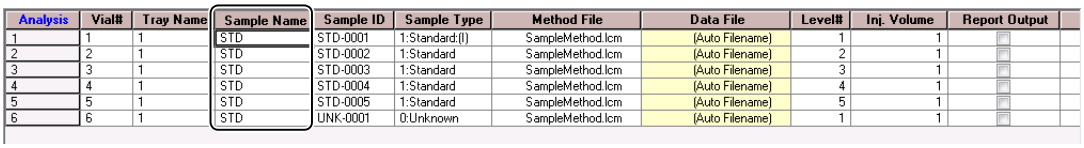


| Analysis | Vial# | Tray Name | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# | Inj. Volume | Report Output |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | STD | STD-0001 | 1:Standard:(I) | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |
| 2 | 2 | 1 | Standard Sample | STD-0002 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 2 | 1 | |
| 3 | 3 | 1 | Standard Sample | STD-0003 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 3 | 1 | |
| 4 | 4 | 1 | Standard Sample | STD-0004 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 4 | 1 | |
| 5 | 5 | 1 | Standard Sample | STD-0005 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 5 | 1 | |
| 6 | 6 | 1 | Unknown Sample | UNK-0001 | 0:Unknown | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |

**2** **Right-click the top cell of the [Sample Name] column that is to be copied, and click [Fill Down].**




The contents of the top cell is copied to the subsequent cells of the [Sample Name] column.

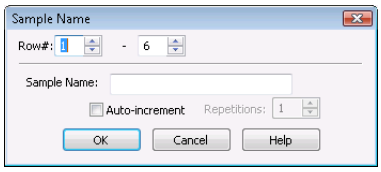


| Analysis | Vial# | Tray Name | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# | Inj. Volume | Report Output |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | STD | STD-0001 | 1:Standard:(I) | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |
| 2 | 2 | 1 | STD | STD-0002 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 2 | 1 | |
| 3 | 3 | 1 | STD | STD-0003 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 3 | 1 | |
| 4 | 4 | 1 | STD | STD-0004 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 4 | 1 | |
| 5 | 5 | 1 | STD | STD-0005 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 5 | 1 | |
| 6 | 6 | 1 | STD | UNK-0001 | 0:Unknown | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |

### [Fill Down]

[Fill Down] functions according to how the cell is selected.

- If only 1 cell is selected (ex: “STD”)
  All selected cells following the selected cell become STD.
- If multiple cells are selected (ex: “STD1”, “AAA” and “STD5” are selected in this order)
  All cells become the same STD1 as the initial cell.
- If a blank cell is selected (ex: a cell in the [Sample Name] column)
  The [Sample Name] sub-window opens. Enter the [Sample Name] parameters, and click [OK].




## 3.2.3 Batch Table Parameters

In addition to sample information and sample type, method file, data file, and report output settings, the following Batch Table parameters can also be set.

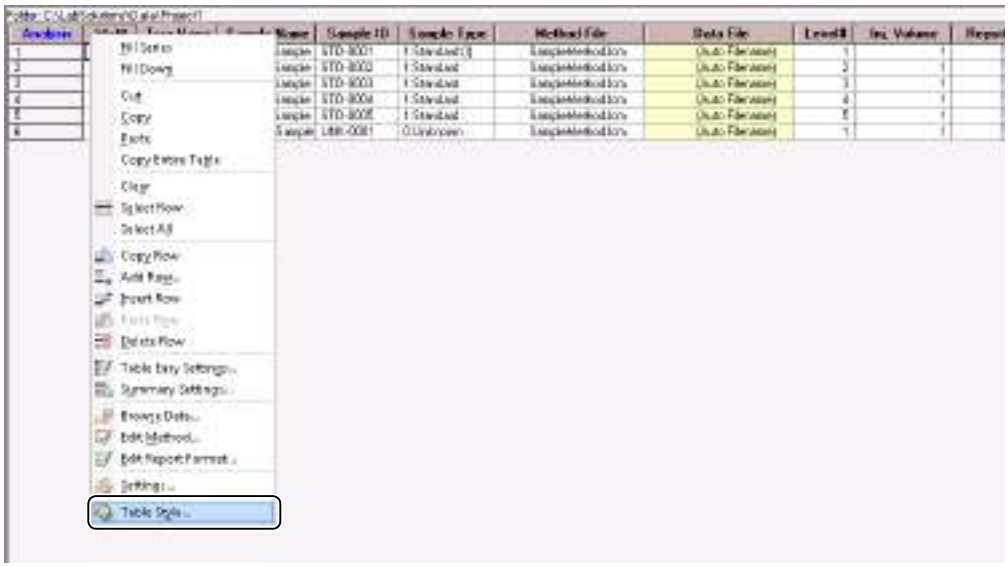
| Parameter | Contents |
|---|---|
| Run mode | Determines whether there is a standby period before data acquisition, and whether to execute data acquisition and data processing on each row of the Batch Table. |
| Background compensation | Performs compensation using the blank (solvent only) chromatogram to subtract baseline drift or solvent peaks.<br>**Reference**<br>For details, refer to *"3.4.5 Background Data File" P.63*. |
| System check | Performs a system check before data acquisition, enter the system check parameter in the top row of the Batch Table. Click the [System Check] cell, and enter the system check parameters in the [System Check] sub-window. |
| System suitability | Checks the suitability of the system based on the analysis results of known multiple samples.<br>The results can be displayed or output in text format. |
| Custom parameters | Calculation formulas can be set for totaling the peak area of related substances in analysis data and for compensating quantitative values. The results are output to a Quantitative Results Table or reports.<br>**Reference**<br>For details, refer to *"3.4.7 Custom Calculation Function" P.65*. |
| Action | The batch processing can be controlled according to pass/fail of the check conditions in each row of the Batch Table. |
| Options 1 to 10 | Up to ten additional information columns can be added to the Batch Table.<br>Once you enter [Option Title] in <Settings> - [Option Items] Tab, this additional sample information is saved in the same data as [Sample Name] and [Sample ID]. |

## ■ Hide or Display Batch Table Items

Use the [Table Style] sub-window to hide or display columns in the Batch Table.

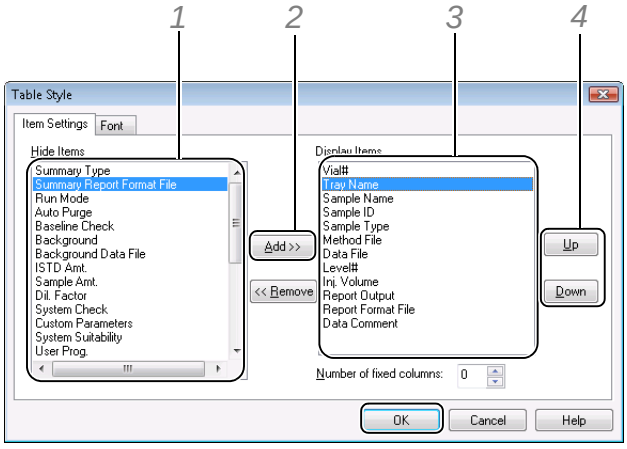
This section describes how to add or delete displayed items to the Batch Table.

**1** **Right-click on the Batch Table, and select [Table Style].**



**2** **Select the desired items, and click [OK].**

### Display Hidden Batch Table Items




1 Select the items to display from the [Hide Items] list.

2 Click [Add].

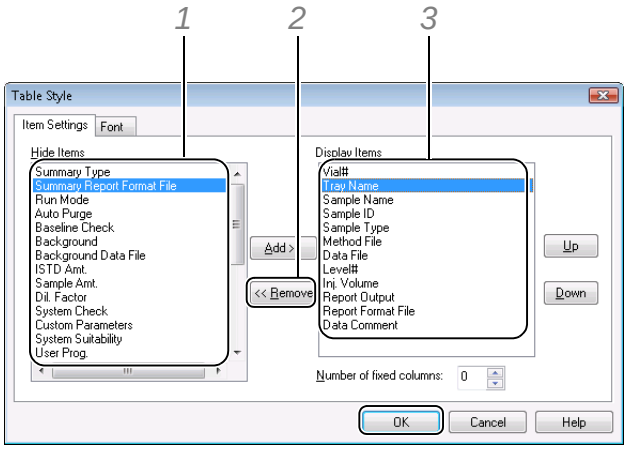
The selected items are added to the end of the [Display Items] list.

3 Select an item to change the display order.

4 Click [Up] or [Down].

The top item in the [Display Items] list is displayed in the first (left) Batch Table column.

## Hide Items in the Batch Table




1 Select the items to hide from the [Display Items] list.

2 Click [Remove].

The selected items move to the [Hide Items] list.

**NOTE**

Realtime batch is executed based on settings in the Batch Table even if the items are hidden. For example, if a summary report output and summary report format file are entered, the summary report is output after realtime batch ends even if these items are hidden in the Batch Table.

# 3.3 Data Acquisition Using Batch Tables

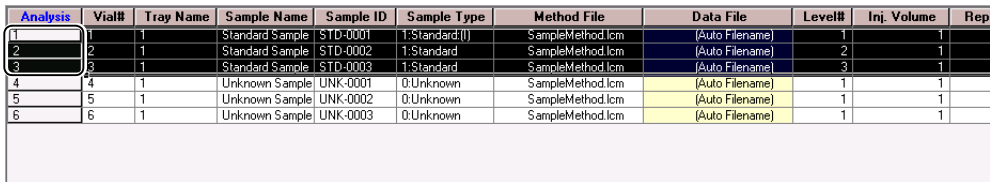
Perform data acquisition using the Batch Table created in *"3.2 Create Batch Tables"*.

This section describes partial execution of a Batch Table, how to stop realtime batch, and how to pause realtime batch to edit the Batch Table.

## 3.3.1 Partial Execution of a Batch Table

This section describes how to perform data analysis on only part of the Batch Table (1 to 3 rows).

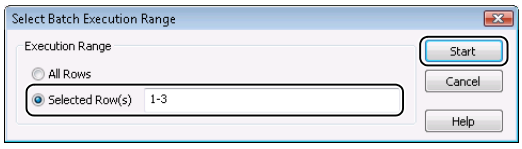
**1** **Select the row numbers to be analyzed.**



| Analysis | Vial# | Tray Name | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# | Inj. Volume | Rep |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | Standard Sample | STD-0001 | 1:Standard(I) | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |
| 2 | 2 | 1 | Standard Sample | STD-0002 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 2 | 1 | |
| 3 | 3 | 1 | Standard Sample | STD-0003 | 1:Standard | SampleMethod.lcm | (Auto Filename) | 3 | 1 | |
| 4 | 4 | 1 | Unknown Sample | UNK-0001 | 0:Unknown | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |
| 5 | 5 | 1 | Unknown Sample | UNK-0002 | 0:Unknown | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |
| 6 | 6 | 1 | Unknown Sample | UNK-0003 | 0:Unknown | SampleMethod.lcm | (Auto Filename) | 1 | 1 | |

**2** **Click the (Start Realtime Batch) icon on the [Realtime Batch] assistant bar.**

**3** **Check [Selected Row(s)], and click [Start].**




A screen for confirming partial execution opens.

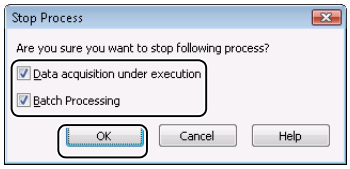
**4** **In this screen, click [OK].**

Batch processing of the selected rows is executed.

## 3.3.2 Stop Realtime Batch

**1** **Click the (Stop) icon on the [Realtime Batch] assistant bar.**


**2** **Select the processes to stop, and click [OK].**




Batch processing is stopped.

**NOTE**

- If only [Data acquisition under execution] is selected, the current data acquisition is stopped and processing moves to the next row of the Batch Table, and data acquisition is started on that row.
- If only [Batch Processing] is selected, processing for the entire Batch Table stops after the current data acquisition ends.
- If both [Data acquisition under execution] and [Batch Processing] are selected, Batch Table processing stops in the middle of the current acquisition.
- When data acquisition is resumed in the row after the stop of batch processing, some information such as, pass/fail information for the QA/QC function, may be cleared.

## 3.3.3 Pause Realtime Batch to Edit the Batch Table

Realtime batch can be paused and the non-acquired rows of the Batch Table can be edited (add, insert, delete).

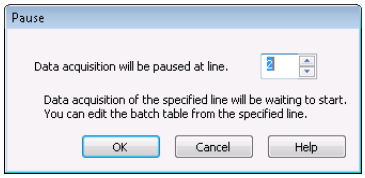
This section describes how to delete a non-acquired row of the Batch Table.

**NOTE**

This operation cannot be performed on rows that have already been acquired.

**1** **During realtime batch, click the (Edit Table/Restart) icon on the [Realtime Batch] assistant bar.**

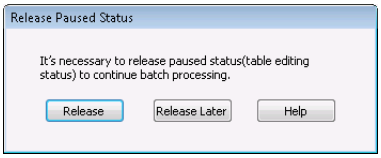
**2** **Set the row where realtime batch is to be paused, and click [OK].**



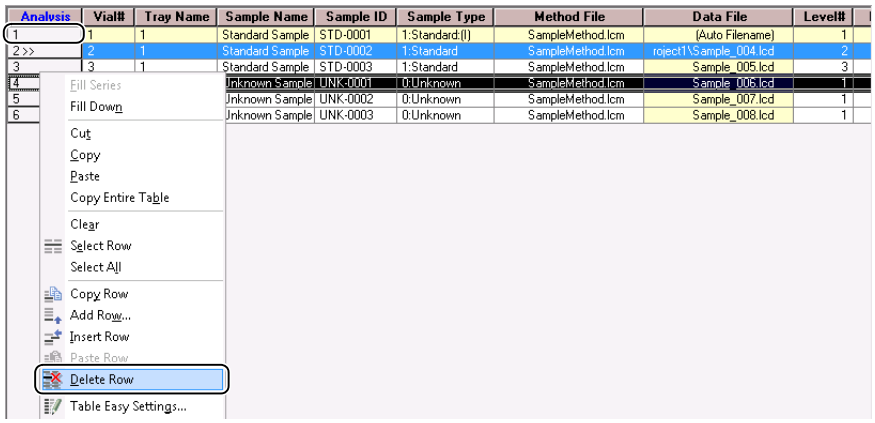

Data acquisition goes into the standby state at the selected row, and batch processing is paused.

**NOTE**

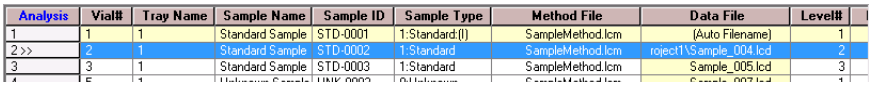
Data acquisition continues until the row selected in the [Pause] sub-windows reached. The [Release Paused Status] sub-window opens when the pause is executed.



**3** **Select the row to be deleted on the Batch Table, right-click on the selected row, and click [Delete Row].**




The selected row is deleted.




**4** **Click the (Save) button on the toolbar.**

The method file is overwritten and saved.

**5** **Click the (Edit Table/Restart) icon on the [Realtime Batch] assistant bar.**

Batch processing is resumed from the paused row.

# 3.4 Automation of Data Acquisition Operations

Using the Batch Table to automate data acquisition allows for the automation of baseline check, system check, startup and shutdown as well as mobile phase substitution (autopurge).

This section describes how to automate data acquisition, output of summary reports, background compensation, bracket quantitation, and the custom calculation function.

**NOTE**
Use the Batch Table [Action] function to control batch processing actions.

## 3.4.1 Check Baseline Stability Before Data Acquisition (Baseline Check)



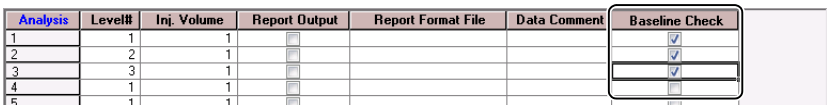
This section describes how to check the baseline before starting data acquisition. Set the baseline check thresholds and other items in the baseline check parameter of the method file.

**NOTE**
The baseline check cannot be performed for MS detectors.

**1** **Select [Baseline Check] in the row where baseline check is to be performed.**

**Reference**

If [Baseline Check] is not displayed in the Batch Table, refer to *"Display Hidden Batch Table Items" P.53*.




**2** **Click the (Save) button on the toolbar.**

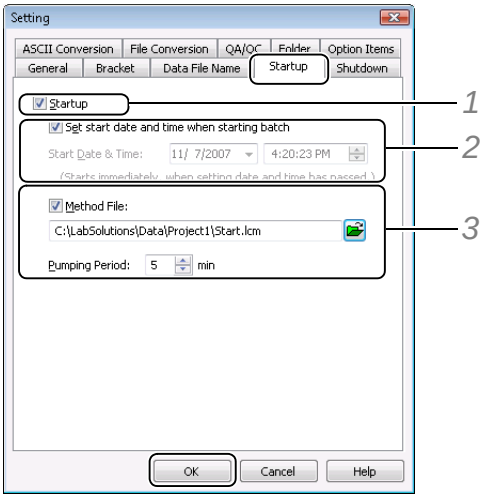
The baseline check settings are saved to the batch file.

## 3.4.2 Start Data Acquisition at a Specified Date and Time (Startup)

Use realtime batch Startup to automatically start realtime batch at a preset date and time. This section describes how to use Startup.

**1** **Click the (Settings) icon on the [Realtime Batch] assistant bar.**

**2** **Click the [Startup] tab, enter the conditions for automatically starting the analytical instruments, and click [OK].**




*1* Select [Startup].

*2* When [Set start date and time when starting batch] is selected, the sub-window for entering the start date and time is displayed.

The analytical instruments are started at the specified [Start Date & Time].

*3* Select [Method File], and enter the name of the method file that contains the parameters for analytical instruments startup.

- Click  to change the referenced file.
- Enter a time in [Pumping Period] for the analytical instruments to operate at the initial conditions before batch processing begins.
- If a method file is not specified, the analytical instruments are started up by the parameters downloaded to the instruments when the startup is performed.

**3** **Click the  (Save) button on the toolbar.**

The startup settings are saved to the batch file.

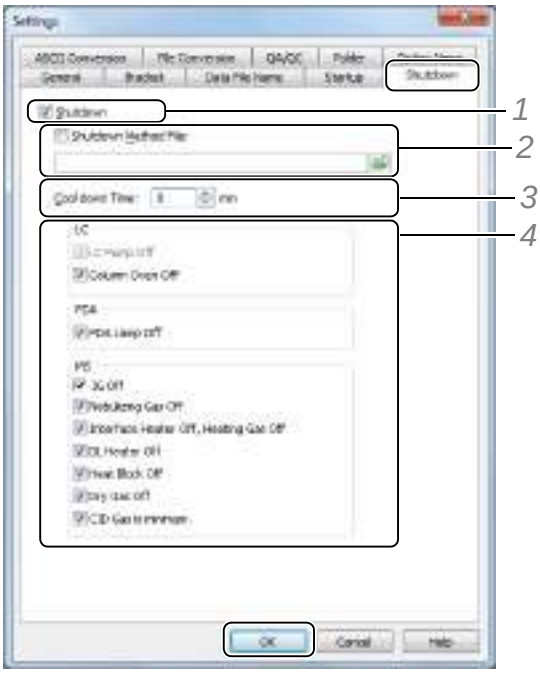
## 3.4.3 Shutdown Analytical Instruments After Data Acquisition (Shutdown)

Use realtime batch Shutdown to automatically shut down the analytical instruments after realtime batch ends. This section describes how to use Shutdown.

**1** **Click the  (Settings) icon on the [Realtime Batch] assistant bar.**

## 2 Click the [Shutdown] tab, enter the conditions for automatic shutdown of the analytical instruments, and click [OK].

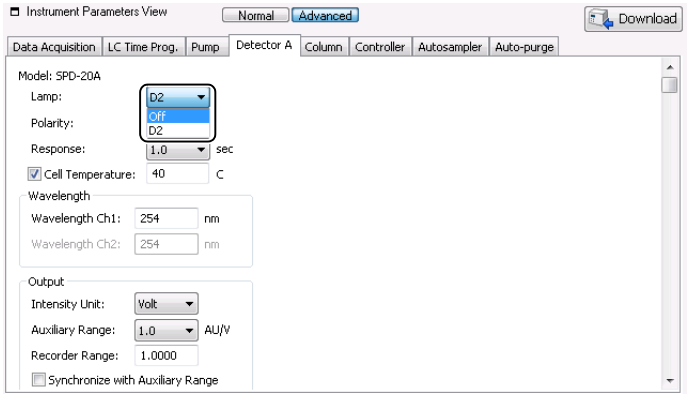
For example: LCMS-8045/8050/8060




1 Select [Shutdown].

2 Select [Shutdown Method File], and enter the name of the method file that contains the parameters for shutdown of the analytical instruments.

- Click  to change the referenced file.
- If a method file is not specified, the analytical instruments are shut down by the parameters downloaded to the instruments when a shutdown is performed.
- When creating a shutdown method file for turn the LC detector lamp off, select [Off] in the [Lamp] parameter.




3 Enter a time in [Cool Down Time] for the instruments to run after analysis and before shutdown.

4 Select the instruments for shut down.

- The displayed items vary according to the MS detector model.

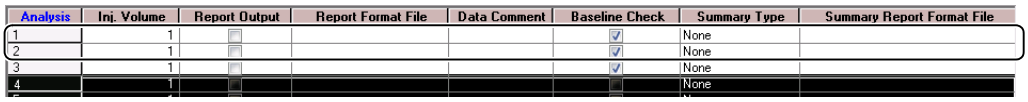
## 3 Click the (Save) button on the toolbar.

The shutdown settings are saved to the batch file.

## 3.4.4 Print a Summary Report

A summary report summarizes the chromatograms and the statistical calculation results from multiple data. This section describes how to set a summary report.

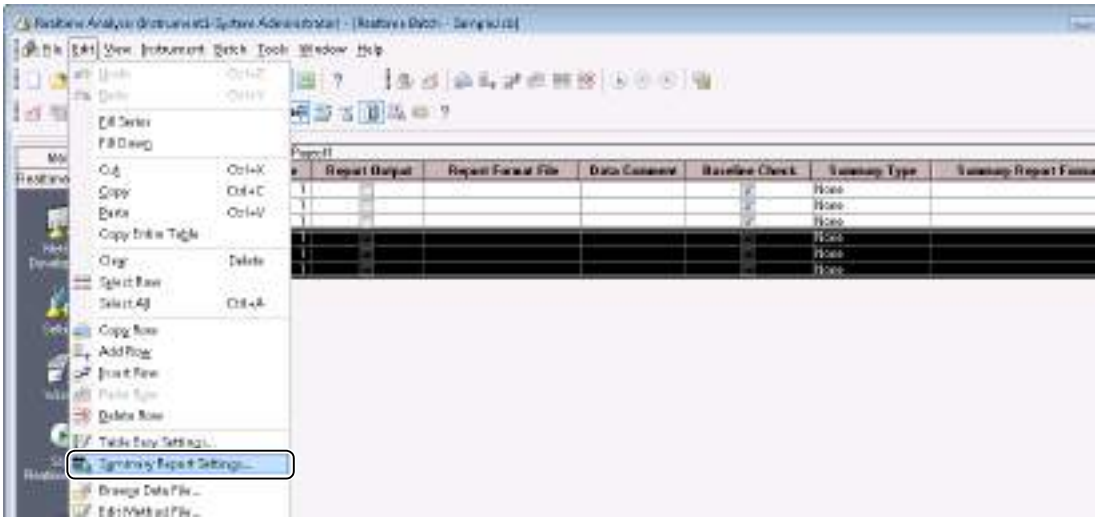
### 1 Drag and select the rows in the Batch Table to be included in the summary report.




**NOTE**

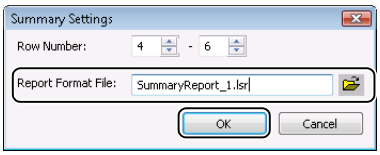
If the [Summary Type] and [Summary Report Format File] items are not displayed in the Batch Table, refer *" Display Hidden Batch Table Items" P.53*.

### 2 Right-click on the selected rows, and click [Summary Report Settings].



### 3 Select a [Report Format File], and click [OK].

- Click  to change the referenced file.
- The selected start row and end row numbers are displayed at [Row Number]. Change the numbers to change the rows to be printed in the summary report.




**Reference**

See *"7.4 Create a Report Format File" P.253* for details on the report format.

### 4 Click the  (Save) button on the toolbar.

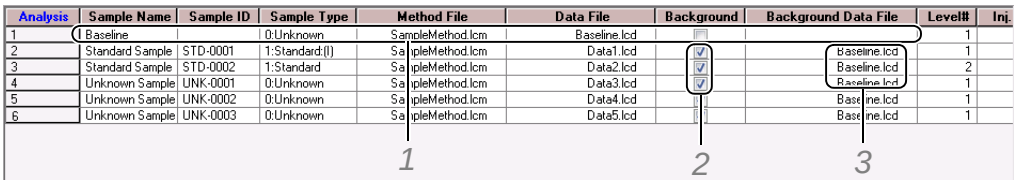
The summary report settings are saved to the batch file.

## 3.4.5 Background Data File

**NOTE**
The function cannot be performed for MS detectors.

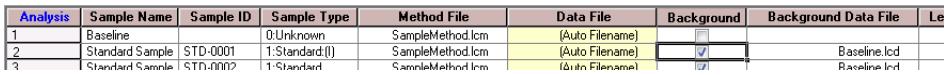
Background data refers to a chromatogram obtained by performing the gradient analysis (LC) without injecting a sample. Use the background data file to compensate for baseline drift in the acquired sample date.

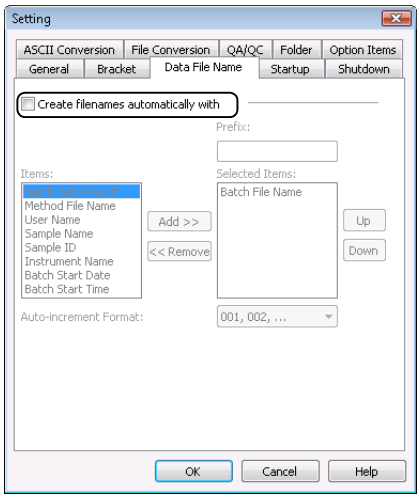
This section describes how to acquire background data and perform background compensation in the same realtime batch.




1 Select the row where background data will be acquired.

**NOTE**
- Ensure that the background data row is above the sample rows.
- If [Auto Filename] is selected for the [Data File] column, click the (Settings) icon on the [Realtime Batch] assistant bar, and select [Create filenames automatically with] on the [Data File Name] tab.




2 Select [Background] for the rows where background compensation will be applied.

3 Enter a [Background Data File] for each of the rows where [Background] is selected.

**Reference**
If [Background] and [Background File] are not displayed in the Batch Table, refer to *"Display Hidden Batch Table Items" P.53*.

**5 Click the (Save) button on the toolbar.**

The background compensation settings are saved to the batch file.

## 3.4.6 Bracket Quantitation

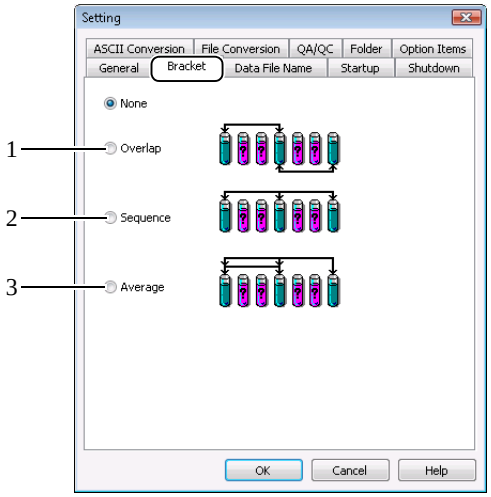
When sequential data acquisition is performed on multiple samples, the detector sensitivity may change over time and sometimes affect the initial and final data acquisition results. To correct this situation, the quantitative value for unknown samples can be obtained by bracketing the unknown sample with standard samples, and creating a calibration curve from the standard sample data acquired before and after the unknown sample.

Three different types of bracket calibration curves are available, [Overlap], [Sequence] and [Average]. Select the appropriate type according to how the standard sample calibration points are set.

This section describes how to select bracket quantitation.

**1** **Click the (Settings) icon on the [Realtime Batch] assistant bar.**

**2** **Click the [Bracket] tab, select the bracket quantitation type, and click [OK].**




| No. | Parameter | Explanation |
|---|---|---|
| 1 | Overlap | Quantitates the unknown sample using the calibration curve made from the results of the standard samples acquired before and after the unknown sample. |
| 2 | Sequence | Quantitates the unknown sample using the calibration curve made from the results of all standard samples regardless of the position of the bracketed unknown sample. |
| 3 | Average | Quantitates the unknown sample using the calibration curve made by averaging the results of all standard samples before the unknown sample and the results of the standard sample directly after the unknown sample. |

**3** **Click the (Save) button on the toolbar.**

The bracket quantitation settings are saved to the batch file.

## 3.4.7 Custom Calculation Function

The custom calculation function allows for automation of operations, such as totaling of the peak area and quantitative value compensation.

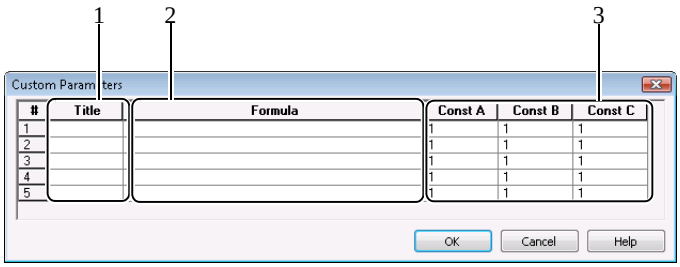
This section describes how to set custom parameters.

**1** **Click the [Custom Parameters] cell in the Batch Table where custom calculations are necessary.**

**Reference**

If the [Custom Parameters] column is not displayed in the Batch Table, refer to *"Hide or Display Batch Table Items" P.53*.

**2** **Enter [Title], [Formula] and constants to display in the Compound Result Table, and click [OK].**



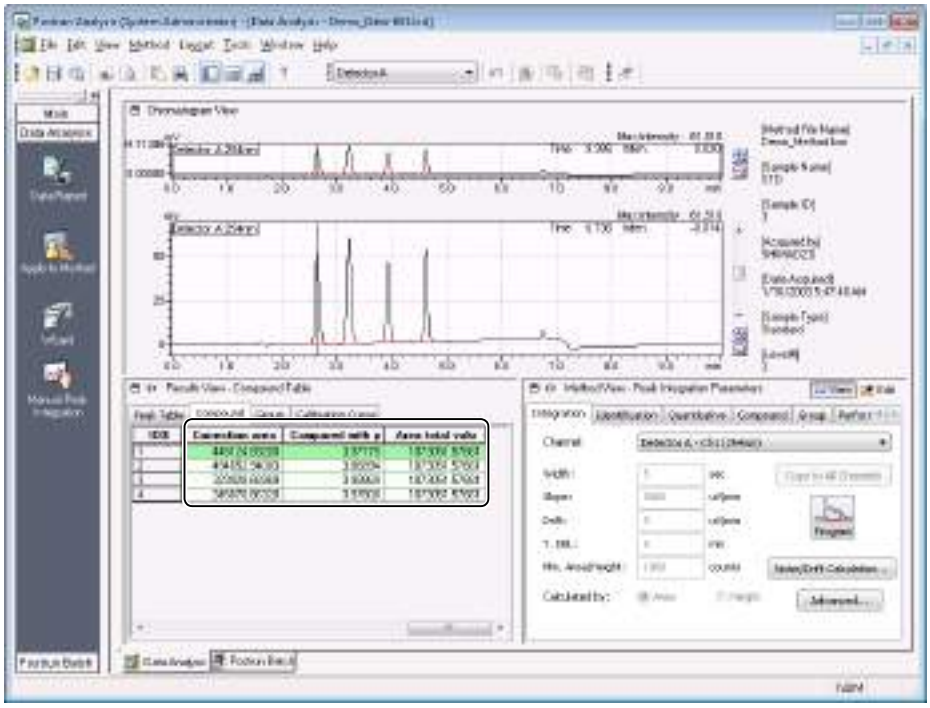

| No. | Parameter | Explanation |
|---|---|---|
| 1 | Title | Enter a title to displayed in the Compound Result Table. |
| 2 | Formula | Enter a formula using numeric values, macro variables and operators (+, -, *, /, e).<br>• Macro variables<br>Retention time (RetTime), area (Area), height (Height), concentration (Conc), Measured retention time of ISTD in the same ISTD group (RetTimeISTD)*, Set retention time of ISTD in the same ISTD group (RetTimeCompTableISTD)*, Set retention time of each compound (RetTimeCompTable)*<br>*: Variables only effective by MS<br>• For a specific peak<br>RetTime [1] (retention time of peak with compound ID “1”)<br>• To specifying peaks between data<br>RetTime [1] (3) (retention time of peak with compound ID “1” of data at 3 rows above the preset row) |
| 3 | Const A to C | Up to any three constants can be specified in each calculation formula. |

**3** **Click the  (Save) button on the toolbar.**

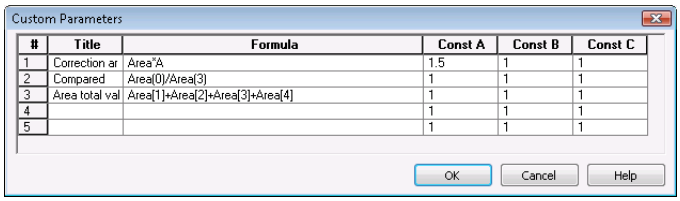
The custom parameter settings are saved to the batch file.

**NOTE**

Execute batch processing to check the calculation results, and then check the results on the [Compound] tab in [Results View]. If custom parameters are not displayed, display them using the [Table Style] sub-window.



### ■ Custom Parameter Example




The 1st row is an example of a compensated area calculation. In this example, each peak area of the unknown sample is multiplied by the compensation factor to obtain the compensated area.

The 2nd row is an example of a calculation between samples. In this example, calculation uses the peak area of an unknown sample and the peak area of a standard sample that was acquired three samples before the unknown sample.

The 3rd row is an example of calculation between peaks. In this example, the total value of 4 peak values is calculated.

## 3.5 Data Acquisition Using the Batch Queue Function

This software allows you to perform continuous data acquisition using different batch files. Batch files used for continuous data acquisition are registered to a memory area called the “batch queue”.

In the batch queue, registered batch files are displayed as a list, and are executed in order by realtime batch from the top of the queue.

The order of registered batch files can be changed and registered batch files can be deleted from the list.

## 3.5.1 Register Batch Files to the Batch Queue

**1** **Click the (Batch Editor) icon on the [Main] assistant bar.**

**2** **Open the batch file in the [Batch Editor] window.**

**3** **Click the (Queue Batch Run) icon on the [Batch Editor] assistant bar.**

The batch file is added to the batch queue.

**NOTE**

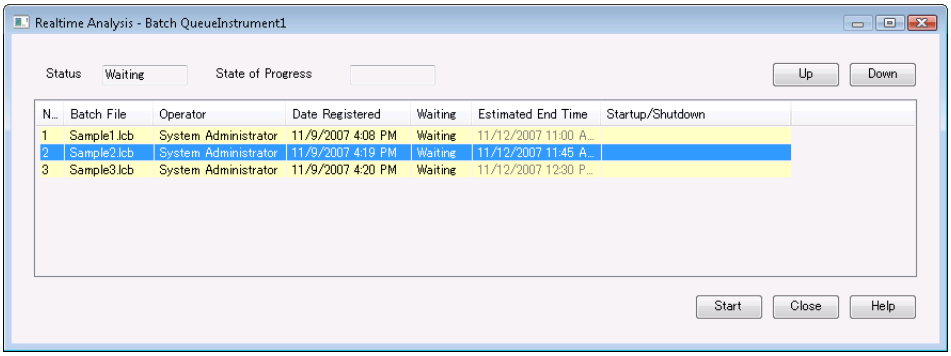
- The information for batch files that are registered to the batch queue is retained even if the [Realtime Analysis] program is exited.
- The status of a batch file registered to the batch queue can be set to “Waiting” (pause) before realtime batch analysis begins on that batch file. Select [The batch queue is registered as a state of “Waiting”] on the [Batch] menu, select the rows of the batch queue to set to the “Waiting” status, and click [Start] to save the batch queue settings.

## 3.5.2 Change the Batch Queue Order or Delete Batch Files

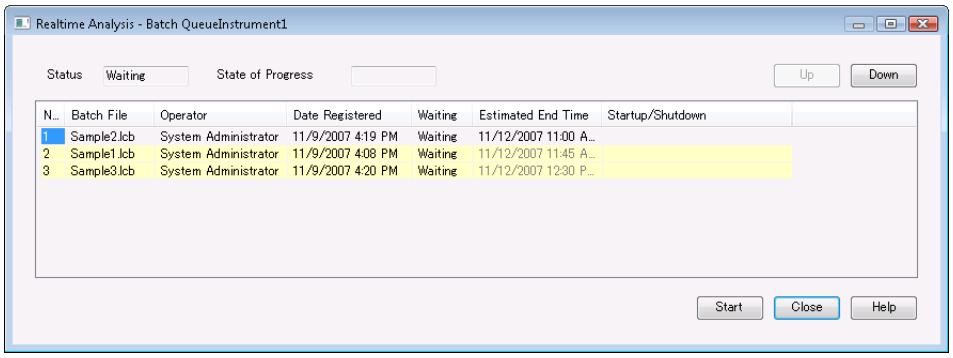
**1** **Click the (Batch Editor) icon on the [Main] assistant bar.**

**2** **Click the (Batch Queue) icon on the [Batch Editor] assistant bar.**

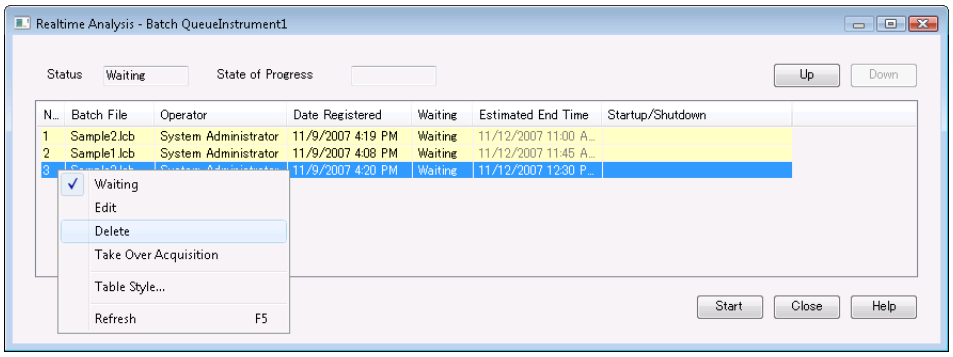
**3** **To change the order of batch files in the batch queue, select the desired row, and click [Up] or [Down].**



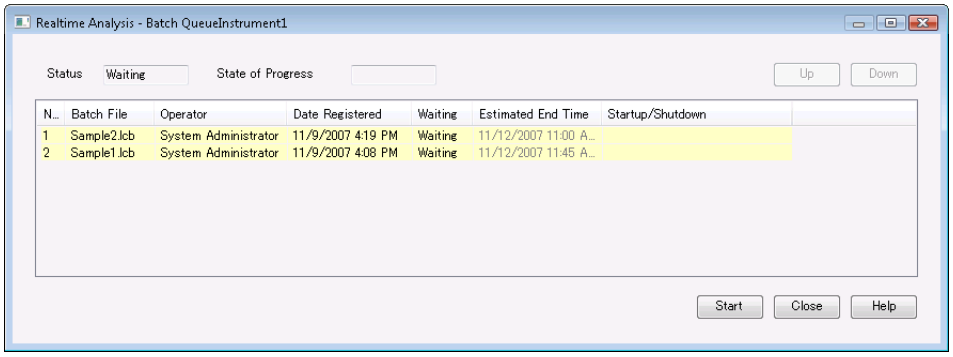
The order of batch files in the batch queue is changed.




## 4 To delete a registered batch file from the batch queue, right-click on the desired row, and click [Delete].




The selected row is deleted from the batch queue.




## 5 Click [Start].

Realtime batch is started in the new batch file order.

## 3.5.3 Priority Batch

The currently acquiring batch file can be paused to give priority to another batch file that must be measured immediately in realtime batch. This is called “priority batch”.

**1** **Click the (Batch Editor) icon on the [Main] assistant bar.**

**2** **Display the batch file to give priority to in realtime batch.**

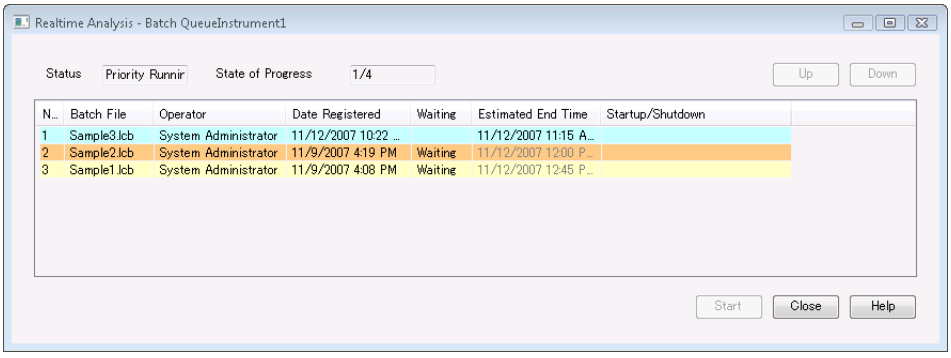
**3** **Click [Start Priority Batch] on the [Batch] menu.**

The priority batch is started.

**NOTE**

- Priority batch is started after the current data acquisition ends.
- Priority batch cannot be set to batch files set with bracket quantitation, summary report, QA/QC, and batch action.

The following shows an example of how the [Batch Queue] sub-window changes when priority batch is set for batch file Sample3.lcb.



# 3.6 Create a Calibration Curve to Quantitate an Unknown Sample

If data processing parameters have already been determined for a target compound, they may be extracted from a method so that a calibration curve can automatically be established during acquisition of standard samples and used for quantitation of unknown samples.

This section describes how to set data processing parameters and Batch Table items to perform quantitative calculations.

## 3.6.1 Edit the Data Processing Parameters

This section describes how to edit the LC data processing parameters.



**1** **Click the (Data Analysis) icon on the [Acquisition] assistant bar.**

**2** **Drag-and-drop the data file onto the [Data Analysis] window from the [Data Explorer] sub-window.**

Select a data file with data acquisition conditions (instrument parameters) that match those for the target component to be analyzed.

**3** **Click the (Wizard) icon on the [Data Analysis] assistant bar.**

**Reference**

Refer to *"6.7 Use the "Compound Table Wizard"" P.232* for MS data.

**4** **Refer to *"4.5.1 Compound Table Wizard" P.116* to set the data processing parameters using the Compound Table Wizard.**

**5** **Click View (View Mode) in [Method View].**

The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the analysis results in [Chromatogram View] and [Results View].

**6** **Click the (Apply to Method) icon on the [Data Analysis] assistant bar.**

The parameters are exported to the method file.

**Reference**

For details, see *"4.7 Save (Export) to Method Files" P.126*.

## 3.6.2 Edit Batch Tables

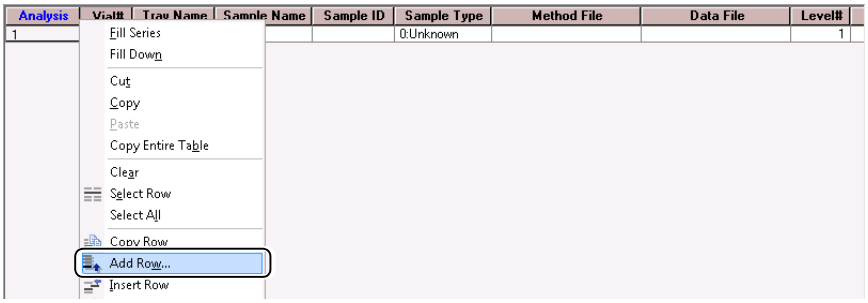
This section describes how to the set the [Method File], [Sample Type], [Level#], [Data File], [Sample Amt.], [Dil. Factor.], and [ISTD Amt.] items required for quantitative calculation.

**NOTE**

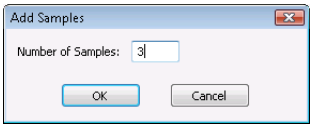
See *"3.2 Create Batch Tables" P.43* for details on other items.

### ■ Add Rows to Batch Tables

**1** **Right-click on the Batch Table, and select [Add Row] from the displayed menu.**




**2** **Enter the number of samples, and click [OK].**




Rows are added to the Batch Table.

| Analysis | Vial# | Tray Name | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# |
|---|---|---|---|---|---|---|---|---|
| 1 | | | | | 0:Unknown | | | 1 |
| 2 | | | | | 0:Unknown | | | 1 |
| 3 | | | | | 0:Unknown | | | 1 |
| 4 | | | | | 0:Unknown | | | 1 |

## ■ Set the Method File

**1** **Click the [Method File] cell on the Batch Table.**

| Analysis | Vial# | Tray Name | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# |
|---|---|---|---|---|---|---|---|---|
| 1 | | | | | 0:Unknown | | | 1 |
| 2 | | | | | 0:Unknown | | | 1 |
| 3 | | | | | 0:Unknown | | | 1 |
| 4 | | | | | 0:Unknown | | | 1 |

**2** **Select the method file, and click [Open].**

The method file is set.

| Analysis | Vial# | Tray Name | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# |
|---|---|---|---|---|---|---|---|---|
| 1 | | | | | 0:Unknown | SampleMethod.lcm | | 1 |
| 2 | | | | | 0:Unknown | | | 1 |
| 3 | | | | | 0:Unknown | | | 1 |

**3** **Set other [Method File] cells in the same way.**

### Reference

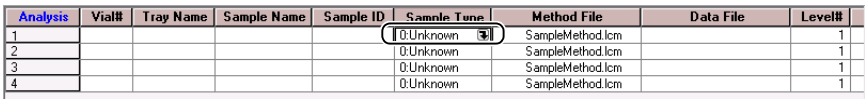
Refer to *"Copy Settings" P.51* to copy and paste the same method file name to multiple rows.

## ■ Set the Sample Type

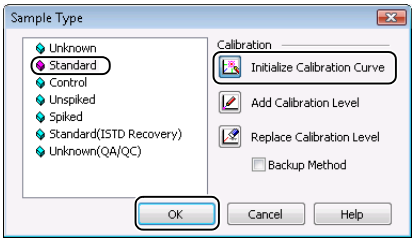
Set the type of sample to measure.

In the case of a standard sample, set the first standard sample to [Initialize Calibration Curve] and the next standard sample to [Add Calibration Level]. The default setting [0: Unknown] is used for unknown samples.

**1** **Click the [Sample Type] cell of the first standard sample.**

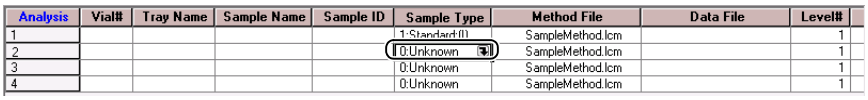



**2** **Click [Standard], select [Initialize Calibration Curve] and click [OK].**

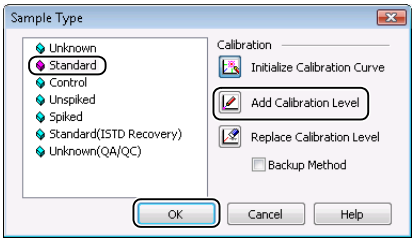



The initial cell for the sample type is displayed as [1: Standard (I)].

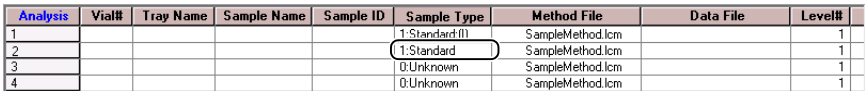
**3** **Click the [Sample Type] cell of the next standard sample.**




**4** **Click [Standard], select [Add Calibration Level] and click [OK].**




The [Sample Type] cell is displayed as [1: Standard].
Repeat steps 3 and 4 for multiple standard samples.



## ■ Set the Level#

Set the standard sample [Level#] according to the concentration value in the Compound Table of the method file. The calibration points are created from the level number of the Compound Table and the area and height values of the preset standard sample.

**NOTE**

[Level#] values are not used for unknown samples, even if they are set.

**1** **Click the [Level#] cell for the standard sample.**

| Analysis | Vial# | Tray Name | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# |
|---|---|---|---|---|---|---|---|---|
| 1 | | | | | 1:Standard:(I) | SampleMethod.lcm | | 1 |
| 2 | | | | | 1:Standard | SampleMethod.lcm | | 1 |
| 3 | | | | | 0:Unknown | SampleMethod.lcm | | 1 |
| 4 | | | | | 0:Unknown | SampleMethod.lcm | | 1 |

**2** **Enter the level number.**

| Analysis | Vial# | Tray Name | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# |
|---|---|---|---|---|---|---|---|---|
| 1 | | | | | 1:Standard:(I) | SampleMethod.lcm | | 1 |
| 2 | | | | | 1:Standard | SampleMethod.lcm | | 4 |
| 3 | | | | | 0:Unknown | SampleMethod.lcm | | 1 |
| 4 | | | | | 0:Unknown | SampleMethod.lcm | | 1 |

The level number is changed.

**3** **Set the [Level#] cell for other standard samples.**

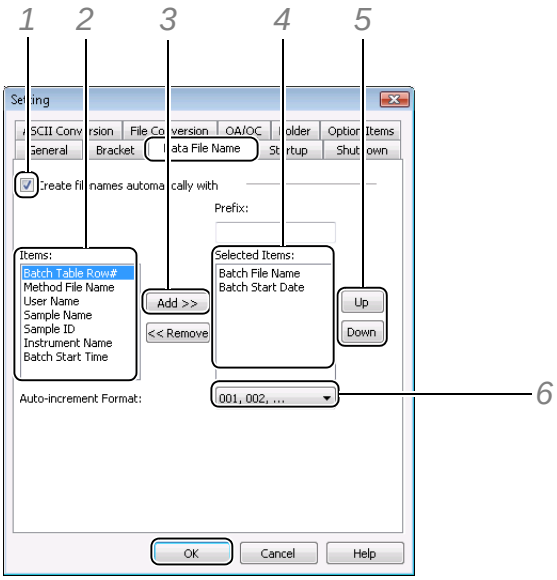
## ■ Set the Data File Name

Either directly enter a file name in the [Data File] cell, or automatically create the data file.

This section describes how to automatically create a data file name.

**1** **Click the (Settings) icon on the [Realtime Batch] assistant bar.**

## 2 Click the [Data File Name] tab, set each item, and click [OK].




1 Select [Create filenames automatically with].

2 Select the items for the file name to automatically create from the [Items] list.

Enter a character string in the [Prefix] box to create a data file name with a fixed character string.

3 Click [Add].

Items are added onto the end of [Selected Items], and the file name is created using the currently displayed items.

4 Select an item in the [Selected Items] list to change the display order.

5 Change the display order by clicking [Up] or [Down].

**NOTE**

Automatically created file names use an _ (underscore) to join together items in order starting with the top item in the [Selected Items] box.
For example, when a file name is automatically created using Batch File Name (AAA), Batch Start Date (2008/04/01):
the file name is “AAA_20080401”.

6 Select a numeric format to automatically append the file name with an incremental number at [Auto-increment Format].

The data file name in the Batch Table is displayed as [Auto Filename].

| Analysis | Sample Name | Sample ID | Sample Type | Method File | Data File | Background | Background Data File | Level# | Inj. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Baseline | | 0:Unknown | SampleMethod.lcm | (Auto Filename) | | | 1 | |
| 2 | Standard Sample | STD-0001 | 1:Standard:(I) | SampleMethod.lcm | (Auto Filename) | ☑ | Baseline.lcd | 1 | |
| 3 | Standard Sample | STD-0002 | 1:Standard | SampleMethod.lcm | (Auto Filename) | ☑ | Baseline.lcd | 2 | |
| 4 | Unknown Sample | UNK-0001 | 0:Unknown | SampleMethod.lcm | (Auto Filename) | ☑ | Baseline.lcd | 1 | |
| 5 | Unknown Sample | UNK-0002 | 0:Unknown | SampleMethod.lcm | (Auto Filename) | ☑ | Baseline.lcd | 1 | |
| 6 | Unknown Sample | UNK-0003 | 0:Unknown | SampleMethod.lcm | (Auto Filename) | ☑ | Baseline.lcd | 1 | |

**NOTE**

Postrun batch reprocessing cannot be executed when a field is set to [Auto-increment Format] because a specific filename and path are required. Therefore, it is recommended to copy the batch after realtime acquisition ends. When a batch is copied, the data file name generated at the time of data acquisition is transferred to the appropriate cell of the copied batch allowing postrun batch processing to be executed.

To copy a batch, select the following menu item.

## ■ Set the Sample Amount, Dilution Factor, and ISTD Amount.

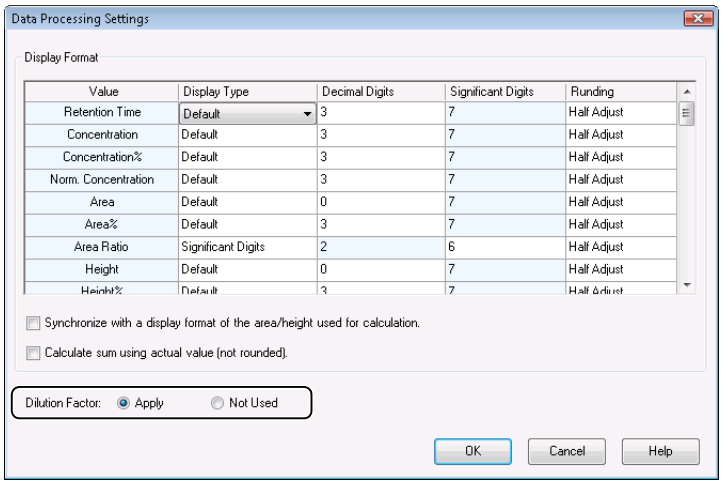
Enter values in each cell of the Batch Table to set the [Sample Amt.] (weight) and dilution factor for an unknown sample, and ISTD amount (for internal standard method) to spike the unknown sample.

This section describes how to set the ISTD amount.



### NOTE

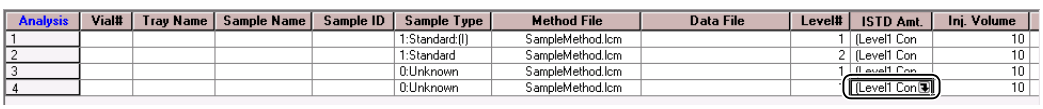
- Enter the ISTD amount for sample types other than the standard sample when the quantitative calculation method is internal standard method.
- Enter the concentration of the ISTD for the number of internal standard substances set in the Compound Table.
- Set [Dilution Factor] to either [Apply] or [Not Used] in the [Data Processing Setting] sub-window in the [System Settings] sub-window.



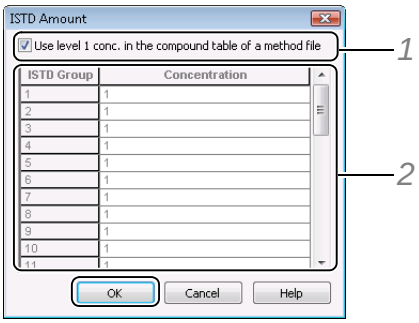

### Reference

If [Sample Amt.], [Dil. Factor] and [ISTD Amt.] are not displayed in the Batch Table, refer to *"Hide or Display Batch Table Items" P.53*.

**1** **Click the [ISTD Amt.] cell for the unknown sample.**



## 2 Enter the concentration for each internal standard substance, and click [OK].




1 Deselect [Use level 1 conc. in the compound table of a method file].
If [Use level 1 conc. in the compound table of a method file] is selected, the level 1 concentrations of the compounds specified as the internal standard substances in the method file are used. Select this checkbox when a standard sample and unknown sample are spiked with the same amount of internal standard substances.

2 Enter the concentrations of the internal standard substances in each group.

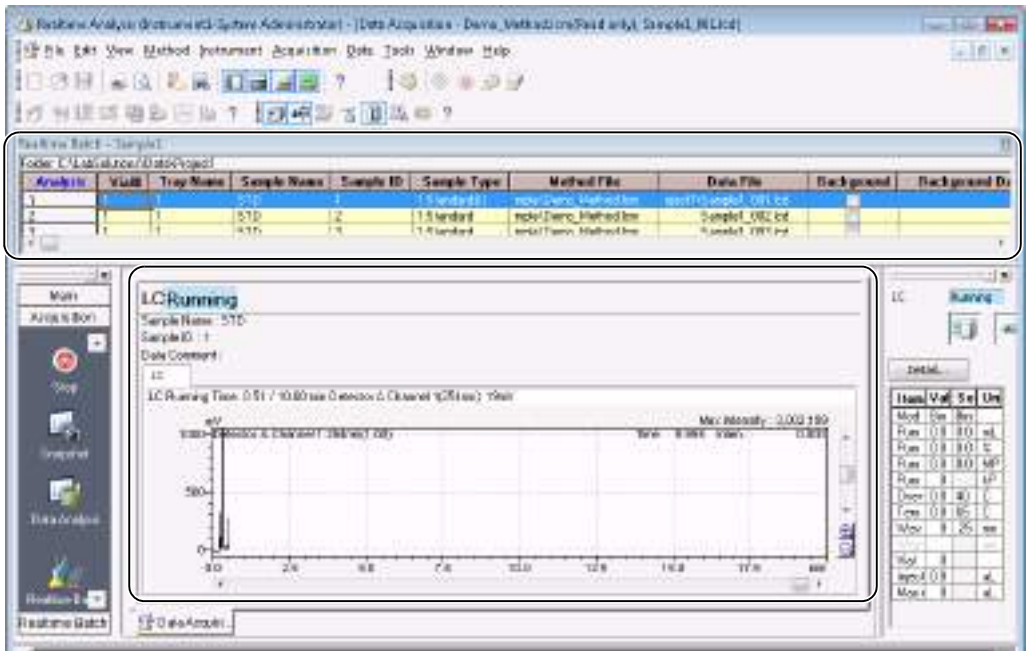
## 3 Enter the [ISTD Amt.] cell for other unknown samples.

## 3.6.3 Data Acquisition Using Batch Tables

Perform data acquisition using a preset batch file.

**1** **Click the (Start Realtime Batch) icon on the [Realtime Batch] assistant bar.**

When data acquisition is started, the [Realtime Batch] and [Data Acquisition] windows change as follows.




During data acquisition, the [LabSolutions Service] icon in the Systray on the Taskbar flashes green.

**NOTE**

Do not turn the PC off while the [LabSolutions Service] icon is flashing.

**Reference**

See *"3.3.2 Stop Realtime Batch" P.56* for details on how to stop or pause realtime batch.

### ■ When an Autosampler Is Not Used

When a manual injector on the LC is connected to the Manual Inject (start) terminals of the system controller, initiate acquisition by rotating the manual injector to the inject position.

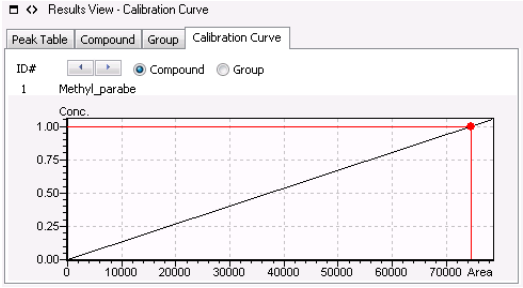
## 3.6.4 Check the Quantitation Results

Check the quantitation results for the unknown sample in the [Data Analysis] window.

**1** **Click the (Data Analysis) icon on the [Realtime Batch] assistant bar.**

The [Postrun Analysis] program is displayed, and the data file for the selected row on the Batch Table is loaded.

**2** **Click the [Compound] and [Calibration Curve] tabs in [Results View], and check the quantitation results.**

# 3.7 Data Acquisition Using the Optimization Function for the Data Acquisition Cycle Time

During realtime batch, the data acquisition cycle can be sped up by overlapping the autosampler operation for the next acquisition before the current acquisition is complete.

**NOTE**

This function is enabled when the CBM-20A/20Alite (Ver. 2.0 or later) is used as the LC system controller. (Any model of autosampler can be used, as long as it can be connected to the CBM-20A/20Alite.)

Both the method file and the batch file must be set in order to use the autosampler overlap operation. This section describes these setting procedures.



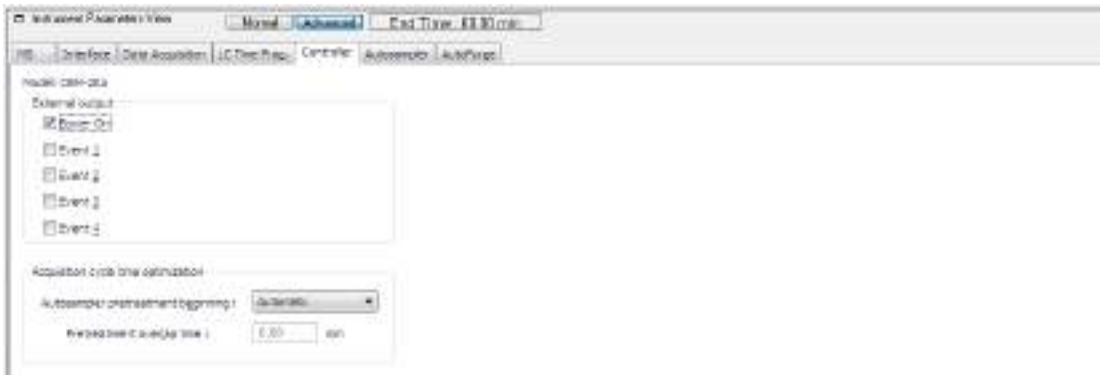
## 3.7.1 Set the Instrument Parameters

**1** **Click the (Data Acquisition) icon on the [Main] assistant bar in the [Realtime Analysis] program.**

**2** **Click [Advanced] in [Instrument Parameter View].**

**3** **Click the [Controller] tab.**

**4** **Select [Automatic] at [Autosampler pretreatment beginning].**



**Reference**

Refer to Help for details about each of the parameters.

**5** **Select [Save Method File As] on the [File] menu.**

Save the method file.

## 3.7.2 Create Batch Tables

1 **Click the (Realtime Batch) icon on the [Main] assistant bar.**

2 **Open the batch file in the [Realtime Batch].**

3 **Set the method file name saved in *"3.7.1 Set the Instrument Parameters"* in all the rows in the [Method File] column.**

**NOTE**

- Set a method file name in the top row. Then right-click this cell, and click [Fill Down] to fill in all of the rows with the same method file name.
- Overlap injection is not performed between rows with different method file names.

4 **Click the (Settings) icon on the [Realtime Batch] assistant bar.**

5 **Select [Start pretreatment for next sample during current data acquisition] on the [General] tab page.**

**Reference**

Refer to Help for details about each of the parameters.

6 **Save the batch file, and execute realtime batch.**

# 4 Data Analysis

This chapter describes how to display the results of acquired data and set data processing parameters during postrun analysis. The [Data Analysis] window displays the contents of a single data file.

**Reference**

- Use the [Quant Browser] window to display the contents of multiple data files, refer to *"12 Data Browser" P.347*.
- Refer to *"14 LC Calibration Curves" P.391* for details on creating calibration curves used for quantitative calculations.



## 4.1 [Data Analysis] Window

The [Data Analysis] window is comprised of the following views:

- [Chromatogram View] - displays chromatograms and instrument status
- [Results View] - displays Peak Tables and quantitative results
- [Method View] - displays the data processing parameters

### 4.1.1 Open the [Data Analysis] Window

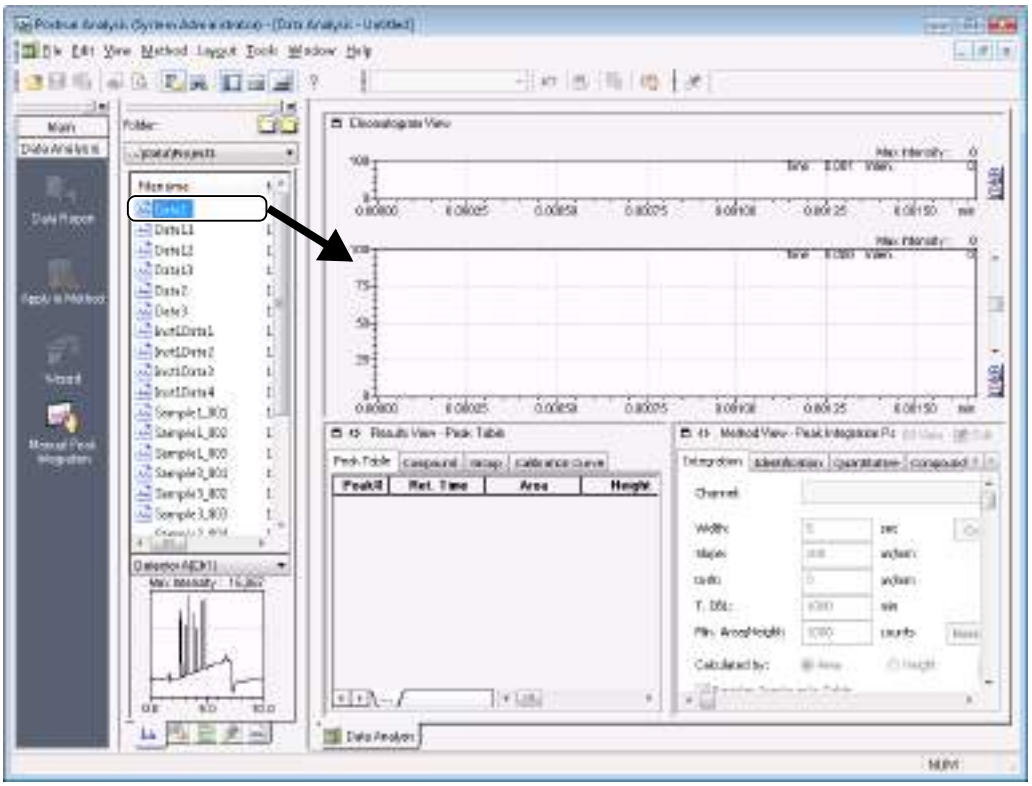
**1** **Click the**  **icon in the [LabSolutions Main] window.**

## 2 Double-click [Postrun].

**NOTE**

The [Data Analysis] window can also be opened by clicking the (Data Analysis) icon on the [Acquisition] assistant bar.

## 3 Drag-and-drop a data file onto the [Data Analysis] window from the [Data Explorer] sub-window.



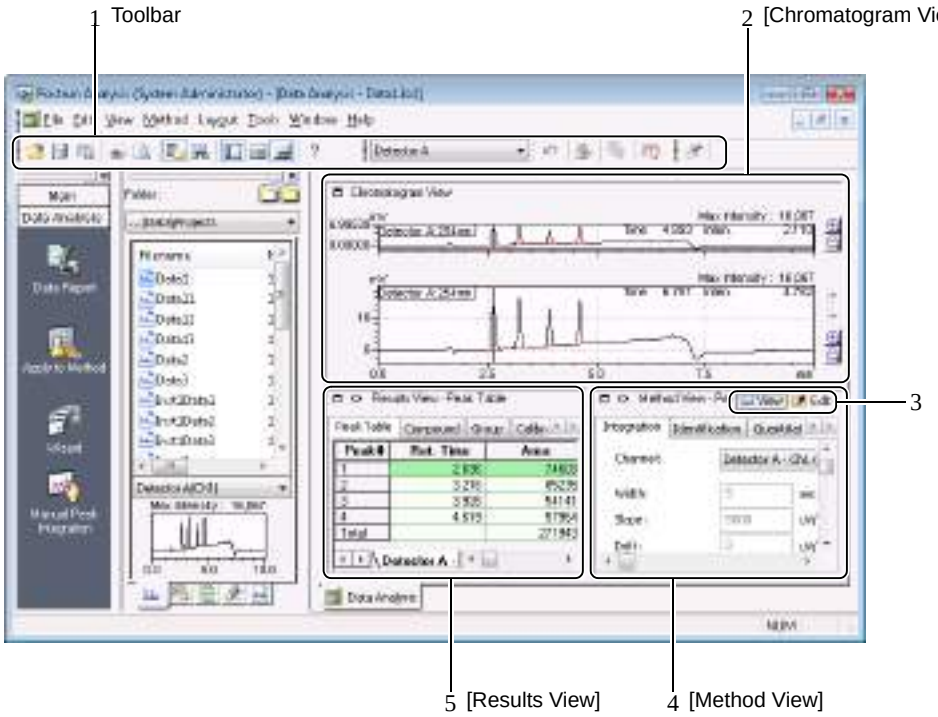
The content of the data file is displayed in the [Data Analysis] window.

## 4.1.2 [Data Analysis] Window Description

This section describes how to view and use the [Data Analysis] window.

**NOTE**

The size of each view can be changed. Click [Save Layout] on the [Layout] menu, and save the changed layout under a new name.



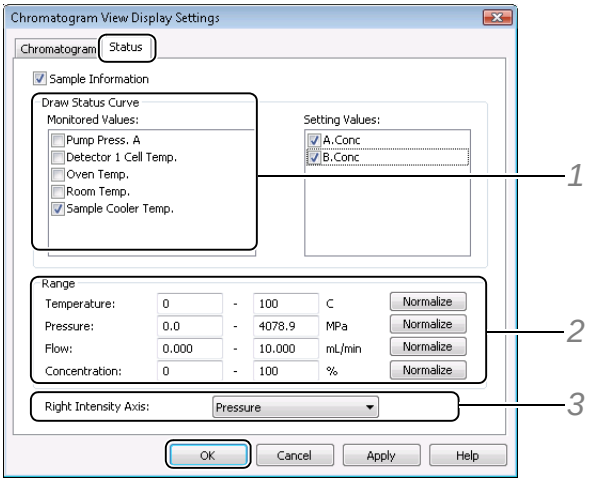

| No. | Explanation |
|---|---|
| 1 | Displays the [Standard] toolbar, [Data Analysis] toolbar, and [Background Compensation Bar]. |
| 2 | Displays the chromatogram for the currently open data file.<br>[Chromatogram View] displays graphs with the [Full Chromatogram] on top and the [Zoomed Chromatogram] on the bottom. If the data has been acquired from multiple detectors, [Other Detector] graphs can also be displayed.<br>[Pressure] and [Flow] can be set to overlaying [Chromatogram View] in the display settings.<br>**Reference**<br>Refer to *"Status Display in the [Chromatogram View]" P.86* for details. |
| 3 | Displays the parameters in the [View] mode.<br>Switch to the [Edit] mode to change the parameters.<br>Change back to the [View] mode to perform postrun analysis using edited parameters. |
| 4 | The data processing parameters are displayed on the [Integration], [Identification], [Quantitative], [Compound], [Group], [Performance], [Custom], and [QC Check] tabs.<br>**Reference**<br>Refer to *"4.2 Peak Integration Parameters" P.88* for details. |
| 5 | The analysis results are displayed on the [Peak Table], [Compound], [Group], and [Calibration Curve] tabs. |

## ■ Status Display in the [Chromatogram View]

The pressure, temperature and other conditions at the time of data acquisition are displayed and can be overlaid in the [Chromatogram View].

**1** **Right-click on the graph, and click [Display Settings].**

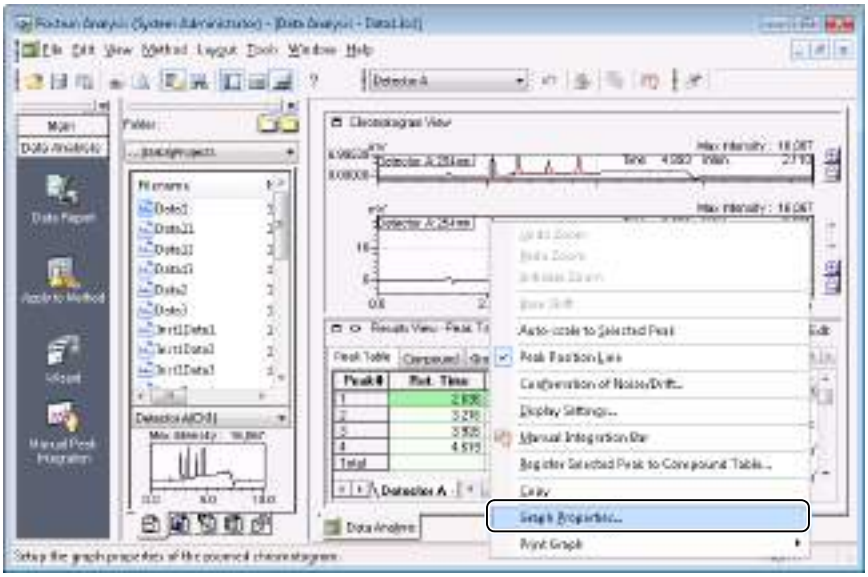
**2** **Click the [Status] tab, make the necessary selections, and click [OK].**



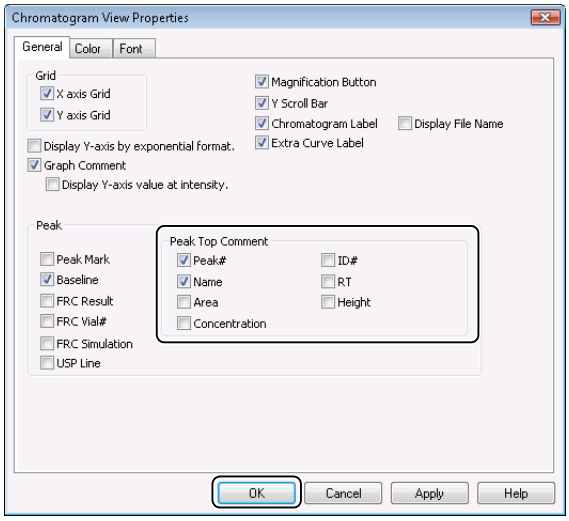

*1* Select the status items to be overlaid on the chromatogram.
*2* Set the display range of each status item or click [Normalize].
*3* Select the parameter to display on the right axis of the graph (Intensity Axis).

## ■ Top of Peak Comment

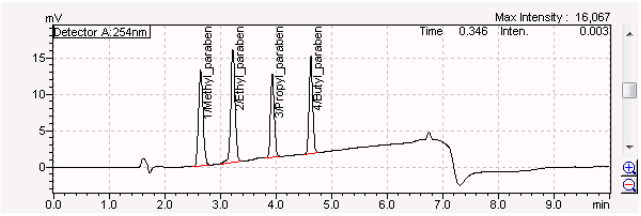
**1** **Right-click on the chromatogram, and click [Graph Properties].**



**2** **Select the peak top comment that is displayed on zoomed chromatograms, and click [OK].**




The selected comment is displayed at the top of the peak in the enlarged chromatogram.



# 4.2 Peak Integration Parameters

Change the peak integration parameters and repeat peak integration.

**NOTE**

While in the [Data Analysis] window, the changes to peak integration parameters are applied only to data processing parameters in the current data file.

The parameters must be exported to a method file before they can be applied to other data, then data processing using this newly saved method must be applied to all of the additional data. Refer to *"4.7 Save (Export) to Method Files" P.126*.

## 4.2.1 Peak Integration of Detected Peaks

This section describes how to set peak integration parameters.

**1** **Click Edit (Edit Mode) in [Method View].**

Click the [Integration] tab, and change the parameters as required.

Click  to change the integration time program and peak selection range.

If analysis was performed on multiple detectors, the parameter changes can be applied to the other channels by clicking [Copy to All Channels].

Click [Noise/Drift Calculation], and make changes to the [Noise/Drift Calculation Settings] in the sub-window that is displayed.

**Reference**

Refer to Help for details about each of the parameters.

**2** **Click View (View Mode) in [Method View].**

The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the processing results in the [Chromatogram View] and [Results View].

## 4.2.2 Remove Unwanted Peak Integration

### ■ Remove Integration of Unwanted Peaks with Minimum Area/Height

Use a larger [Min. Area/Height] value to exclude integration of small peaks.

The following example describes how to change the [Min. Area/Height] value from “1000” to “10000”.

**1** **Click Edit (Edit Mode) in [Method View].**

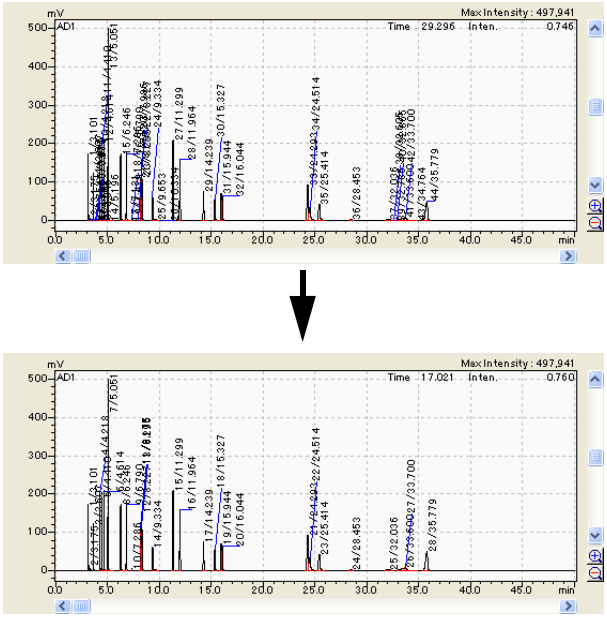
**2** **Click the [Integration] tab, and change the [Min. Area/Height] value to “10000".**

**NOTE**

Select [Height] at [Calculated by] to remove the integration of unwanted peaks based on peak height.

**3** **Click View (View Mode) in [Method View].**

The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the processing results in the [Chromatogram View] and [Results View].



## ■ Remove Integration of Unwanted Peaks with the Integration Time Program

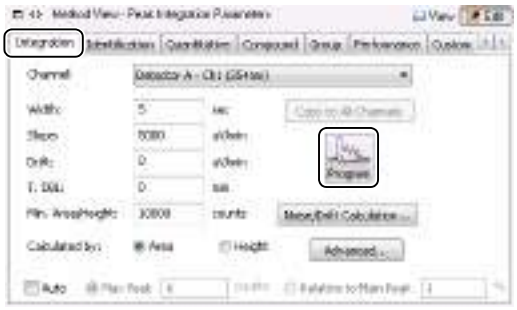
The integration time program allows for detailed peak integration, that is not normally possible with typical integration parameters.

The following example describes how to remove integration of unwanted peaks using the integration time program.

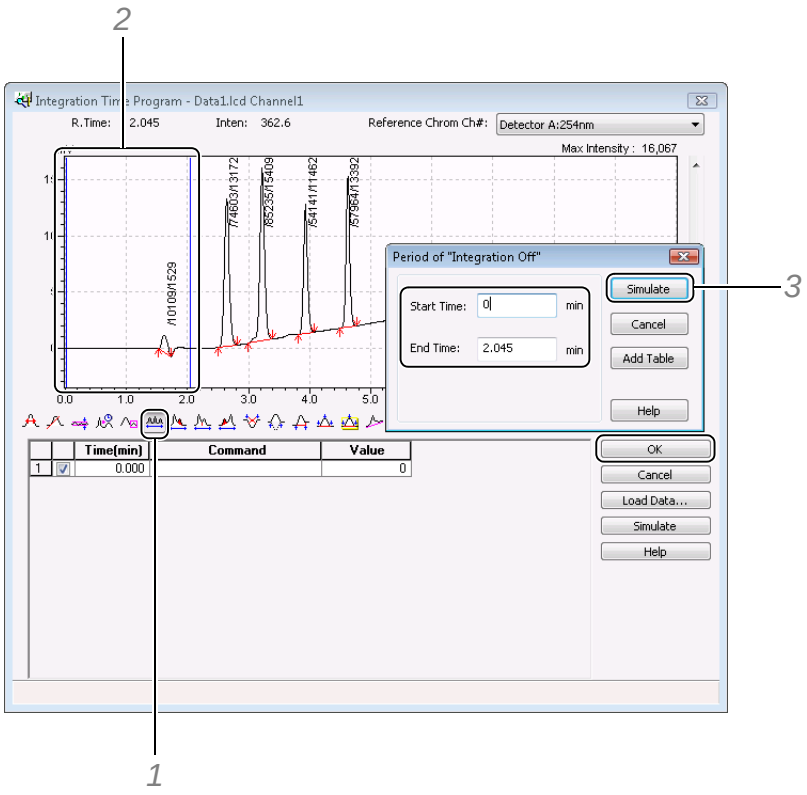
You can delete unwanted peaks by setting a period in which peak detection is not performed in the Time Program Table in the [Integration Time Program] sub-window.

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Integration] tab, and click .**



**3** **Create an integration time program, and click [OK].**

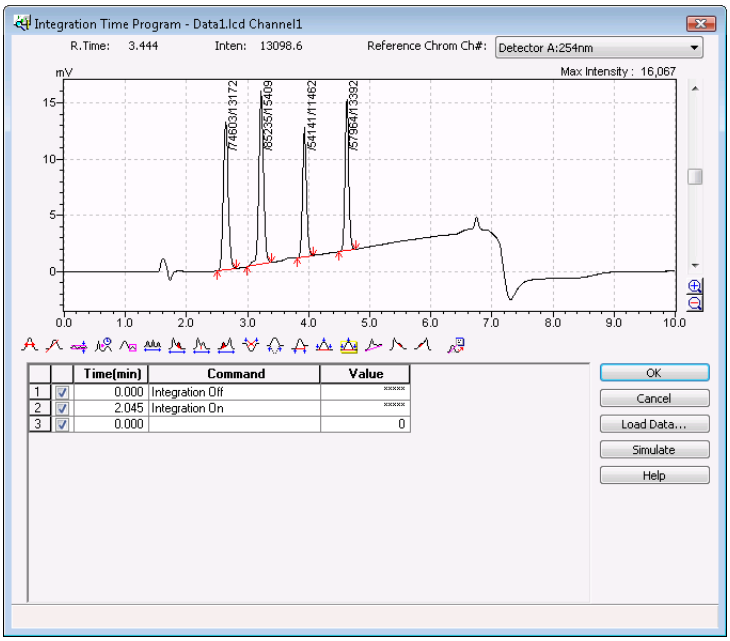



1 Click (Period of “Integration Off”).

2 Use the cursor to select the start and end positions of the range where integration is not performed.

3 Evaluate the [Start Time] and [End Time] in the [Period of “Integration Off”] sub-window, and click [Simulate].

The time and processing commands are added to the time program.
Examine the resulting integration.




**NOTE**

Use the mouse to click to zoom in or out a chromatogram and change the display of the specified view area.

**4** **Click View (View Mode) in [Method View].**

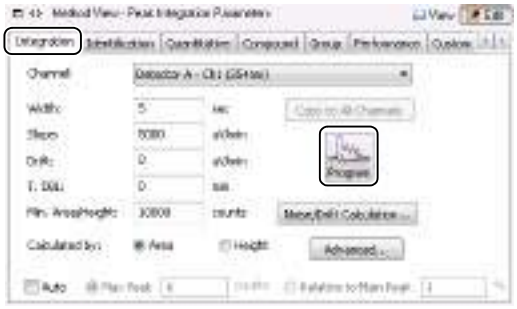
The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the processing results in the [Chromatogram View] and [Results View].

## 4.2.3 Analyze Tailing Peaks

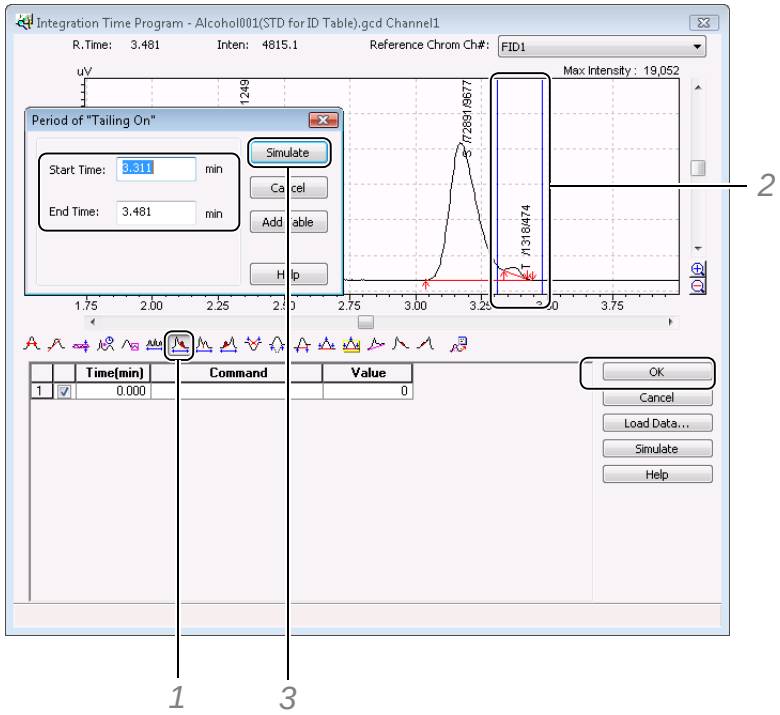
This section describes how to process a target peak that overlays the tail of the main peak.

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Integration] tab, and click .**



## 3 Set the peak to perform tailing processing on, and click [OK].



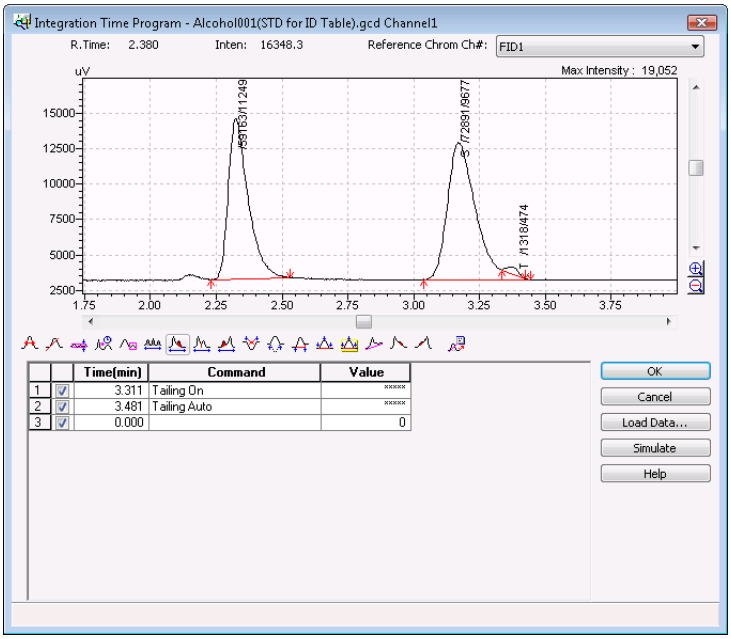

1 Click (Period of “Tailing On”).

2 Use the cursor to select the start and end positions of the range where tailing processing is performed.

3 Evaluate the [Start Time] and [End Time] in the [Period of “Tailing On”] sub-window, and click [Simulate].

The time and processing commands are added to the time program.

Examine the resulting integration.




**NOTE**

If the peak on the tail of the main peak is small, adjust the Slope value until it is detected.

**4** **Click View (View Mode) in [Method View].**

The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the processing results in the [Chromatogram View] and [Results View].

**NOTE**

Referring to the procedure above, click (Period of “Leading On”) if the target peak overlaps the front of the main peak.

## 4.2.4 Manual Peak Integration

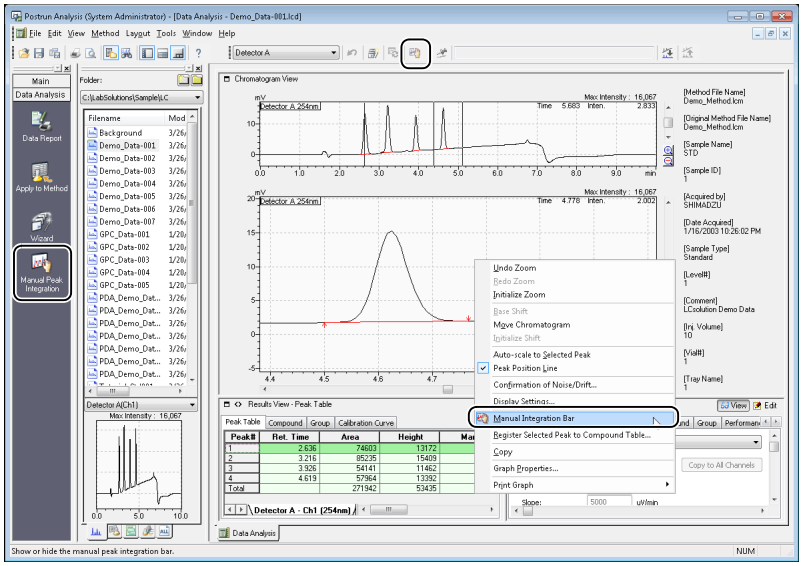
It is possible to manually integrate peaks that are not properly integrated using the automatic integration parameters in the method file.

**NOTE**

- Manual peak integration commands are saved only to current data.
- Manual peak integration commands cannot be exported to the method file.
- To execute the same processing command on multiple data files, make settings in the Integration Time Program in [Method View], and save that method file for use. Alternatively, copy the content in the Manual Peak Integration Table, paste it into other data tables to apply it on them, and then perform analysis.
- The content in the Manual Peak Integration Table is retained even if postrun analysis is performed using the other method files.

### ■ Display [Manual Integration Bar]

**1** **Click the (Manual Peak Integration) icon on the [Data Analysis] assistant bar.**




[Manual Integration Bar] is displayed.

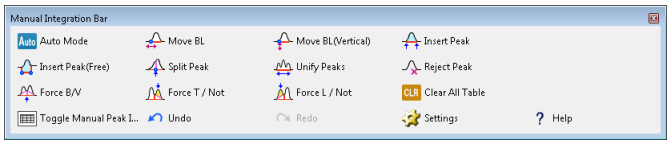
**NOTE**

[Manual Integration Bar] can also be displayed by clicking the (Manual Integration Bar) on the toolbar or right-clicking on [Chromatogram View] and selecting [Manual Integration Bar].

Two types of [Manual Integration Bar] formats are available, Standard toolbar and Advanced toolbar. The format type can be switched by changing the setting.

This section describes the Normal toolbar.

## Manual Integration Bar (Standard Toolbar with Labels)

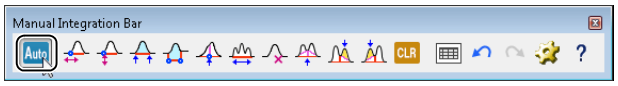



| Icon | Name | Explanation |
|---|---|---|
| | Auto Mode | This mode selects the optimal processing based on the relationship between the position of the mouse cursor and the chromatogram automatically.<br>The command shortcut key can also be used. |
| | Move BL | Moves the peak detection points (start or end) along the X-axis (time). |
| | Move BL (Vertical) | Moves the peak detection points (start or end) along the Y-axis (intensity). |
| | Insert Peak | Inserts a peak start and peak end point for a peak that was not previously integrated. |
| | Insert Peak (Free) | Specifies the times and intensity values of the start point and the end point of the peak, and inserts the peak.<br>A vertically divided peak can be inserted. |
| | Split Peak | Splits a peak vertically at a specified time.<br>If there is a valley near the specified time on the chromatogram, the peak is split at the time on the valley. |
| | Unify Peaks | Unifies two peaks adjacent to a vertical division line that is specified by clicking the mouse. Or, unifies multiple peaks between two points, which are specified by dragging the mouse, into a single peak. |
| | Reject Peak | Removes the peak that is specified by clicking the mouse.<br>Or, removes multiple peaks between two points that are specified by dragging the mouse. |
| | Force B/V | Changes to detection of baseline separation if the separation state of two adjacent peaks is vertical division.<br>Changes to vertical division if the separation state is baseline separation. |
| | Force T / Not | Performs tailing processing if the specified peak is vertically divided. This processes a peak as a peak included in the tailing.<br>If the specified peak is on tailing, vertical division processing is performed. |
| | Force L / Not | Performs leading processing if the specified peak is vertically divided. This processes a peak as a peak included in the leading.<br>If the specified peak is on leading, vertical division processing is performed. |
| | Clear All Table | Deletes all the content in the Manual Peak Integration Table and sets the peak detection method to automatic peak integration. |
| | Toggle Manual Peak Integration Table | Toggles the Manual Peak Integration Table between display/hide. |

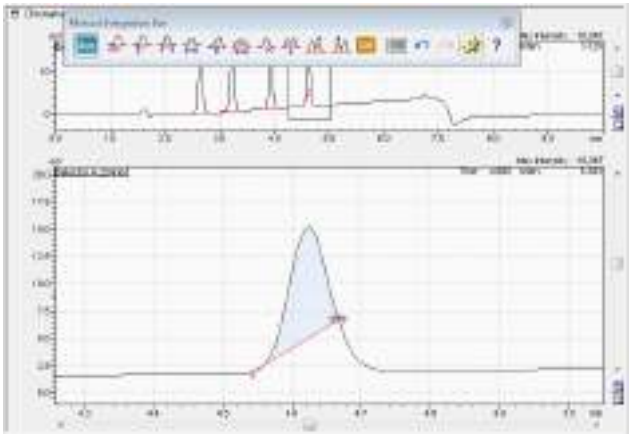
Furthermore, there are three operation types, auto mode, selecting processing commands on the toolbar, and operation by shortcut keys. This section describes operations in auto mode.

## ■ Move the Peak Detection Point in Auto Mode

**1** **Click the Auto (Auto Mode) icon to start the auto mode.**



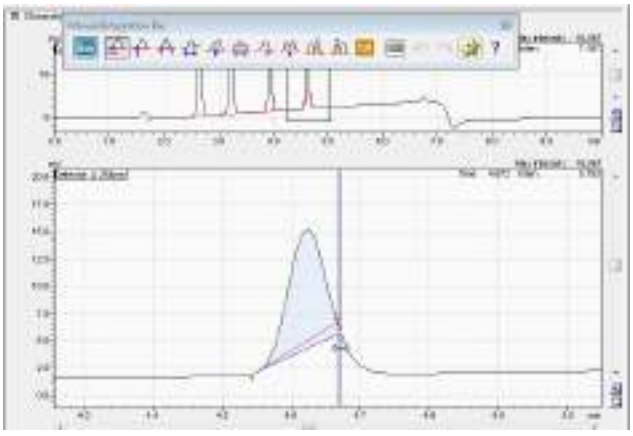

**2** **Move the mouse to near the detection point to move to.**



The detection point is highlighted.

**3** **Click the detection point to move to and confirm it.**

This can be controlled by dragging the mouse.



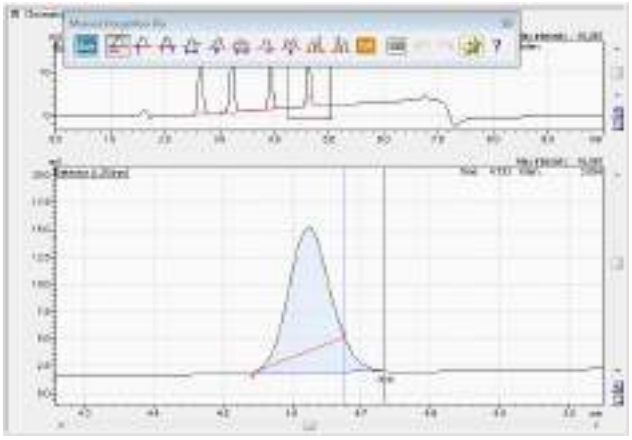
A vertical blue line is displayed.

**NOTE**

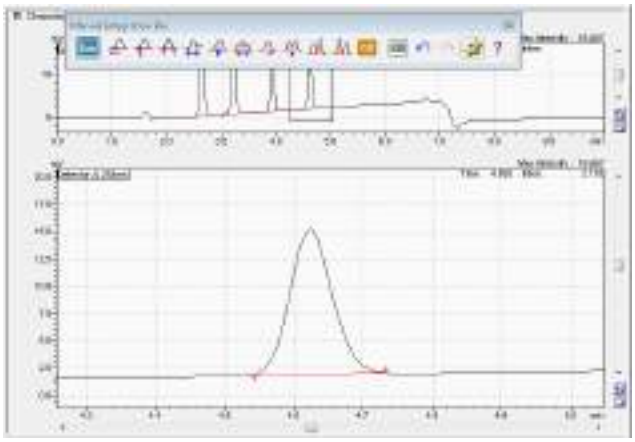
At this time, if the detection point is specified with the [Y] key held down, the point can be moved in the intensity axis direction.

If the point is specified with the [F] key held down, it can be moved in both the X and Y directions.

**4** **Align the mouse (vertical line) to the time of the move destination and click the mouse.**

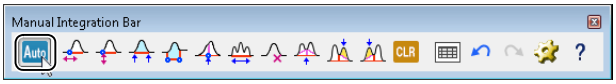


The peak detection point is changed and baseline is adjusted.

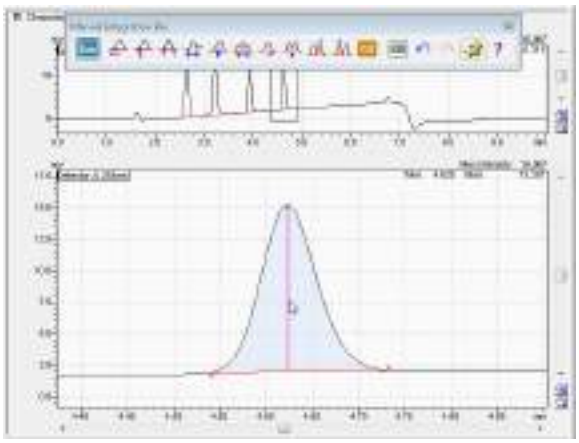


## ■ Remove a Peak in Auto Mode

**1** **Click the**  **(Auto Mode) icon to start the auto mode.**

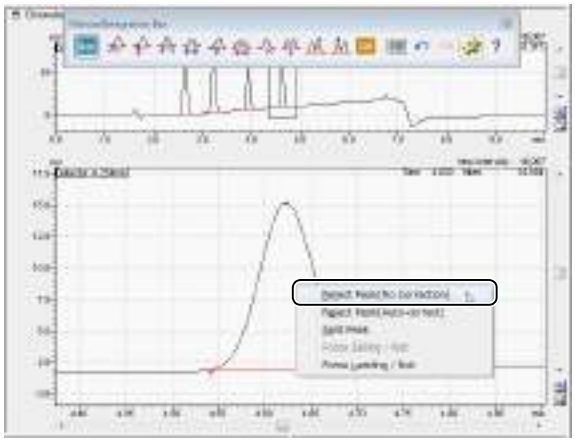


**2** **Move the mouse to inside the peak to remove.**

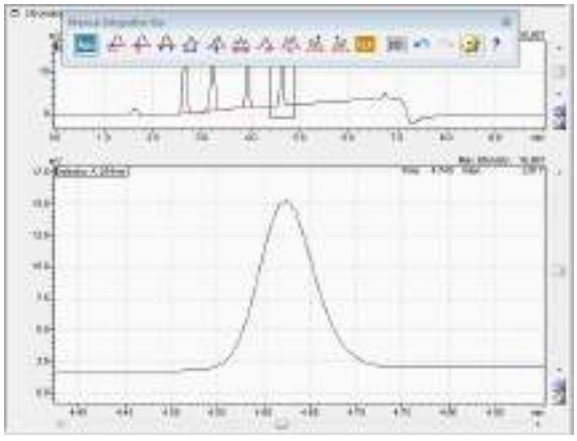


The peak inside is filled.

**3** **Right-click on the graph, and click [Reject Peak(No Correction)] on the displayed menu.**



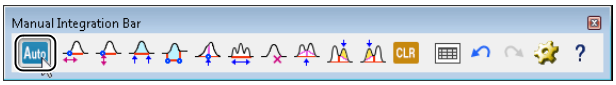
The peak is removed.



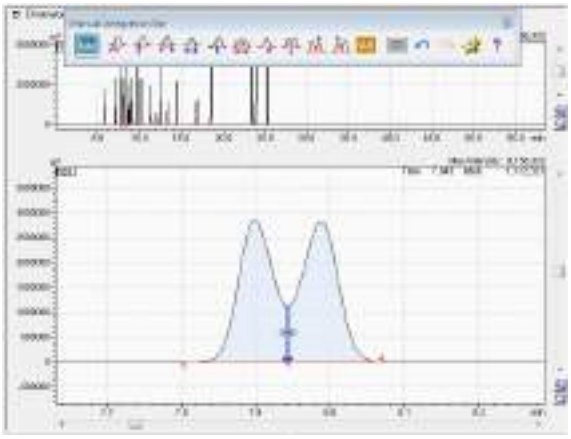
## ■ Unify Peaks in Auto Mode

This section describes how to execute the peak integration processing command on multiple peaks as a single peak.

**1** **Click the (Auto Mode) icon to start the auto mode.**

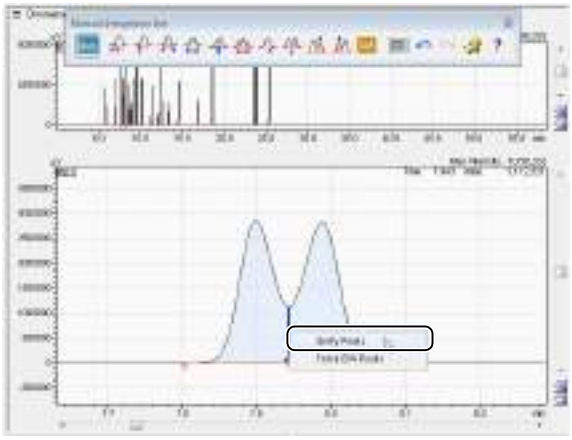



**2** **Move the mouse to near the vertical division line to unify.**

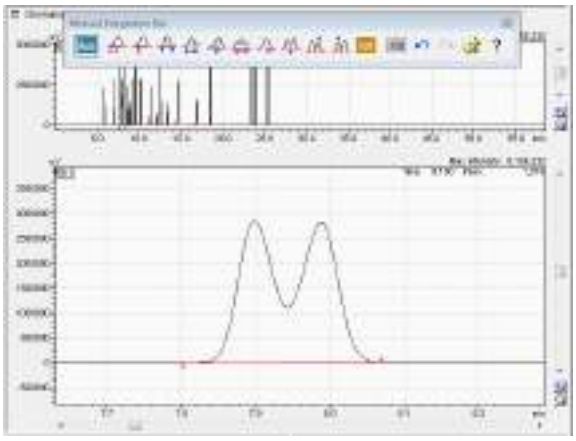


The vertical division line is highlighted.

**3** **Right-click on the graph, and click [Unify Peaks] on the displayed menu.**



The peak is unified.



**NOTE**

The peak integration processing command can also be executed on multiple peaks as a single peak by changing the [Width] value on the [Integration] tab page in [Method View].

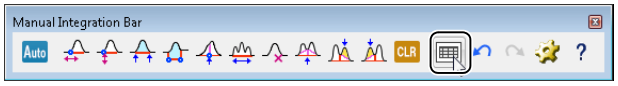
**Reference**

For details on the [Width] value, refer to Help.

## 4.2.5 Enable/Disable Each Processing Command

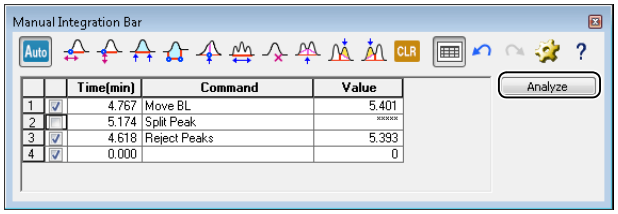
This section describes how to enable/disable each processing command using the Manual Peak Integration Table.

**1** **Click the (Toggle Manual Peak Integration Table) icon on [Manual Integration Bar].**




The Manual Peak Integration Table is displayed.

**2** **Clear the checkbox for the processing command to disable and click [Analyze].**




Only the processing commands with their checkboxes selected are executed again.

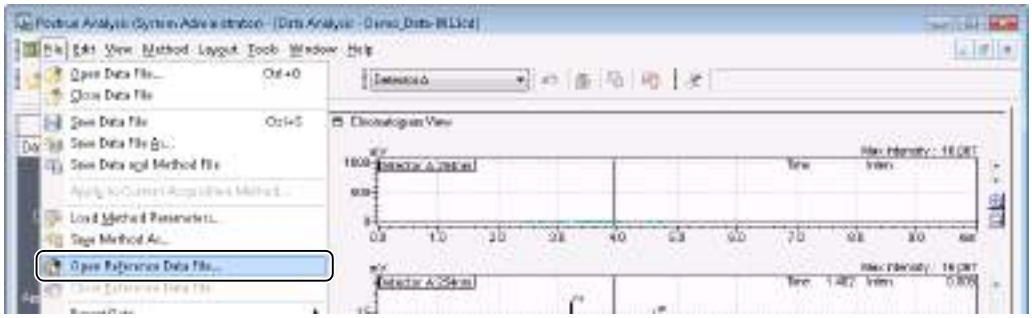
**NOTE**

Pressing the [Delete] key deletes the row selected in the Manual Peak Integration Table.

## 4.2.6 Overlay Data in the Analysis Sub-window

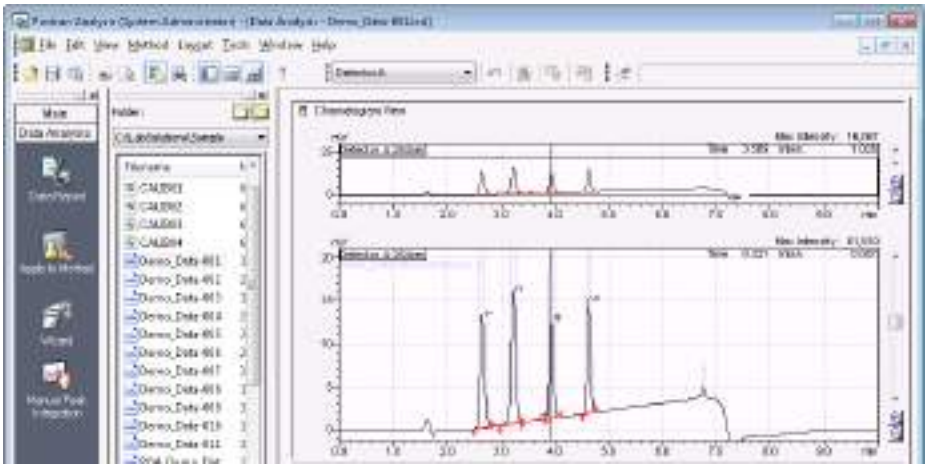
A reference data file can be opened on the current open data file and displayed as an overlay in the [Chromatogram View].

**1** **Select [Open Reference Data File] on the [File] menu.**



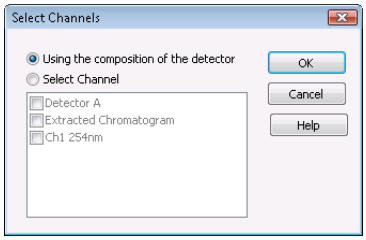
## 2 Click the data file to display, and click [Open].

The chromatogram in the selected data file is displayed on the sub-window.



**NOTE**

- Up to 16 data files can be drawn overlaying each other as reference chromatograms.
- If the data file was obtained by data acquisition on multiple channels, the [Select Channels] sub-window opens to allow for proper chromatogram selection.




- To display the baseline of a reference chromatogram, right-click on the zoomed chromatogram, and select at [Graph Properties].

**Reference**

Refer to *"4.1.2 [Data Analysis] Window Description" P.85* for details.

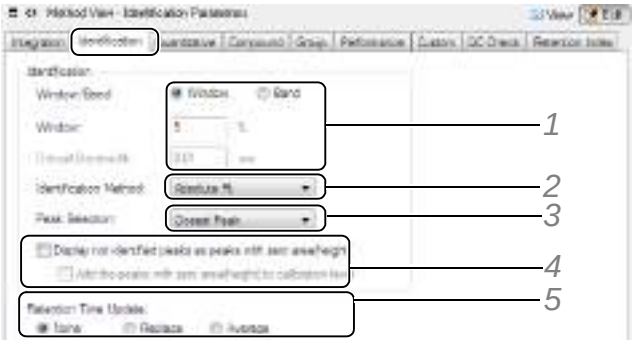
- The peak integration parameters for the reference chromatograms cannot be displayed or modified.

# 4.3 Peak Identification Parameters

This section describes how to set the allowable time width (window/band width) used for identifying peaks based on the Compound Table and which of the identification methods, absolute retention time method or relative retention time method is used.

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Identification] tab, and set each parameter.**




*1* Select either [Window] or [Band] at [Window/Band].
If [Window] is selected, enter [Window] in % units, and if [Band] is selected, enter [Default Band Time] in minutes.

| Parameter | Contents |
|---|---|
| Window | The allowable time width for the peak top is set as a percentage (%) of the retention time. All peaks are calculated with the same window percentage.<br>Allowable time width (min) = ± (Compound Table retention time (min) × window (%) + 0.02) |
| Band | The allowable time width of the peak top is set as an absolute time. The allowable time width can be set to each peak in the Compound Table.<br>Allowable time width (min) = ± Default Band Time (min) |

*2* Select either [Absolute Rt] or [Relative Rt] as the peak identification method.

| Parameter | Contents |
|---|---|
| Absolute Rt | Identifies target peaks from the retention time of each peak and their allowable times preset to the Compound Table. |
| Relative Rt | Compares the retention time of the sample peak to the retention time of the reference peak to compensate for retention time deviation caused by fluctuation of the data acquisition conditions. A reference peak must be set in the Compound Table.<br>**Reference**<br>For details, see *"4.5.4 Directly Edit the Compound Table" P.122*. |

3 Select the peak to identify from [All Peaks], [Closest Peak], and [Largest Peak].

| Parameter | Contents |
|---|---|
| All Peaks | If multiple peaks fall within a single allowable time range, all peaks are identified as the target compound despite whether the Window method or Band method is set as the allowable time width setting method. |
| Closest Peak | If multiple peaks fall within a single allowable time range, only the peak closest to the retention time in the Compound Table is identified as the target compound, despite whether the Window method or Band method is set as the allowable time width setting method. |
| Largest Peak | If multiple peaks fall within a single allowable time range, only the peak with the largest peak area or height value is identified as the target compound, despite whether the Window method or Band method is set as the allowable time width setting method. |
| Similarity | [Similarity] can be selected when the photodiode array detector is used. The similarity between the spectrum at the retention time of the peaks in the allowable identification width and the standard spectrum registered in the Compound Table is calculated, and only the peak with the largest similarity value is identified as the target compound. |

**NOTE**

If peak identification is based on internal standard substances or if peak identification is performed on reference substances, the peak having the maximum area or maximum height is automatically identified regardless of the [Peak Selection] setting.

4 Set [Display not identified peaks as peaks with zero area (height)].

If this checkbox is selected, the information of that compound is displayed at [Results View].

5 Set how the Compound Table retention time is automatically updated based on the retention time of an actually identified peak each time that data processing is performed on the standard sample.

| Parameter | Contents |
|---|---|
| Replace | Replaces the retention time of each compound in the Compound Table with the retention time of the actually identified peak. |
| Average | Replaces the retention time with the value obtained by averaging the retention time of each compound in the Compound Table and the retention time of the actually identified peak. |

## 3 Click View (View Mode) in [Method View].

The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the processing results in the [Chromatogram View] and [Results View].

# 4.4 Quantitative Parameters

This section describes how to set the quantitative parameters used to calculate the concentration values of the target peak.

| Quantitative Processing | Reference |
|---|---|
| Quantitate by external standard method. | *"4.4.1 External Standard Method" P.103* |
| Quantitate by internal standard method. | *"4.4.2 Internal Standard Method" P.105* |
| Quantitate by standard addition method. | *"4.4.3 Standard Addition Method" P.107* |
| Calculate the percentage (%) of each component by corrected area normalization method. | *"4.4.4 Corrected Area Normalization Method" P.109* |
| Quantitate multiple compound peaks as a group | *"4.4.5 Grouping" P.111* |
| Make the calibration curve of the natural logarithmic axis | *"4.4.6 Calibration Curve for Exponential Calculation" P.112* |
| Correct the concentration value of a standard sample using the standard concentration factor. | *"4.4.7 Standard Concentration Factor" P.113* |
| Quantitate using the calibration curve of other components. | *"4.4.8 Reference Standard ID and Correction Factor" P.114* |



## 4.4.1 External Standard Method

This method involves calculating concentrations from the peak area or height of unknown samples using a calibration curve based on a standard sample. This is the most frequently used quantitative calculation method.

Data acquisition is performed on a fixed volume of multiple concentrations of a standard solution that were prepared to bracket the anticipated concentration of the substance in the unknown sample.

A calibration curve is made using the absolute concentration of the standard solution (absolute amount) as the vertical axis and the respective peak area or height as the horizontal axis.
(The X- and Y-axes display can be changed using [X Axis Calib. Curve].)

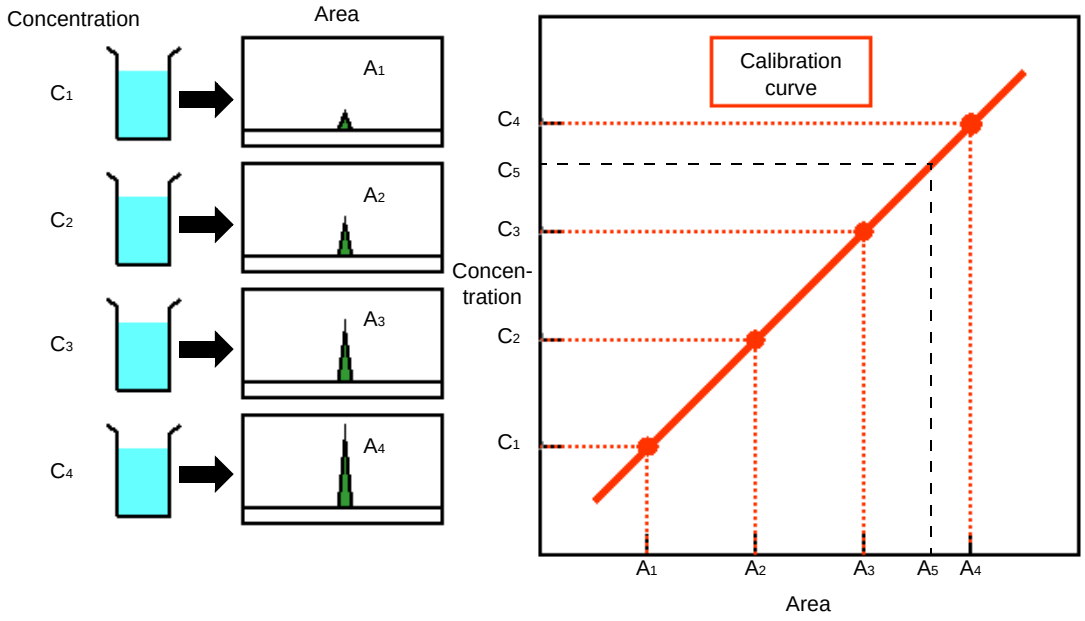



Fig.4-1 External Standard Method (Absolute Calibration Curve Method)

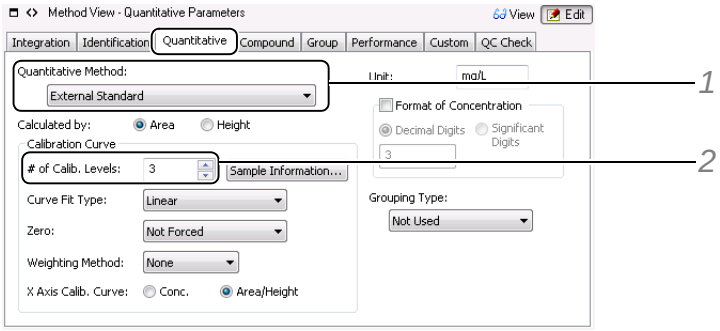
After the calibration curve is created, the same volume of the unknown sample solution is analyzed under the same conditions used to analyze the standard solutions.

The peak area or height (A5) of the unknown sample is determined and the concentration (C5) of the substance in the unknown sample can be calculated from the calibration curve.

This section describes how to quantitate using the “external standard method”.

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Quantitative] tab, and set each parameter.**

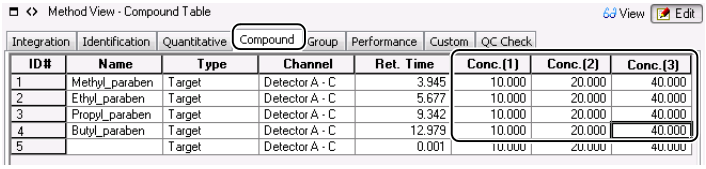



*1* Select [External Standard] for the [Quantitative Method].

*2* Enter the number of concentration levels (calibration points) at [# of Calib. Levels].

**3** **Click the [Compound] tab, and enter the concentration for each of the standard samples in the [Conc. (1)], [Conc. (2)] and [Conc. (3)] columns.**

This example uses a 3-point calibration curve.




| ID# | Name | Type | Channel | Ret. Time | Conc.(1) | Conc.(2) | Conc.(3) |
|---|---|---|---|---|---|---|---|
| 1 | Methyl_paraben | Target | Detector A - C | 3.945 | 10.000 | 20.000 | 40.000 |
| 2 | Ethyl_paraben | Target | Detector A - C | 5.677 | 10.000 | 20.000 | 40.000 |
| 3 | Propyl_paraben | Target | Detector A - C | 9.342 | 10.000 | 20.000 | 40.000 |
| 4 | Butyl_paraben | Target | Detector A - C | 12.979 | 10.000 | 20.000 | 40.000 |
| 5 | | Target | Detector A - C | 0.001 | 10.000 | 20.000 | 40.000 |

**NOTE**

[Not Used] is displayed if the concentration cell is selected and the keyboard [Delete] key is pressed or if “-1” is entered in the cell.

Use this method when separate standard samples are prepared for individual target components.

**4** **Click View (View Mode) in [Method View].**

**5** **Save the method file before creating the calibration curve.**

**Reference**

For details on how to make calibration curves, refer to *"3 Realtime Batch" P.43* or *"14 LC Calibration Curves" P.391*.

## 4.4.2 Internal Standard Method

This highly precise method involves performing quantitative calculation with an area ratio or height ratio to correct for injection volume errors.

The internal standard (ISTD) substance should be a stable compound that separates completely from other peaks in the sample, has a similar chemical nature and elutes near the substance to be quantitated.

The standard solutions are prepared with 1 or more known concentrations of the target substance (“X” from here on) and a specified concentration of the internal standard substance (“ISTD” from here on). Then data acquisition is performed on fixed amounts of these standard solutions.

A calibration curve is created using the ratio of “X concentration/ISTD concentration” in the standard solution as the vertical axis and the ratio of “peak area of X/peak area of ISTD” as the horizontal axis. (The X- and Y-axes display can be changed using [X Axis Calib. Curve].)

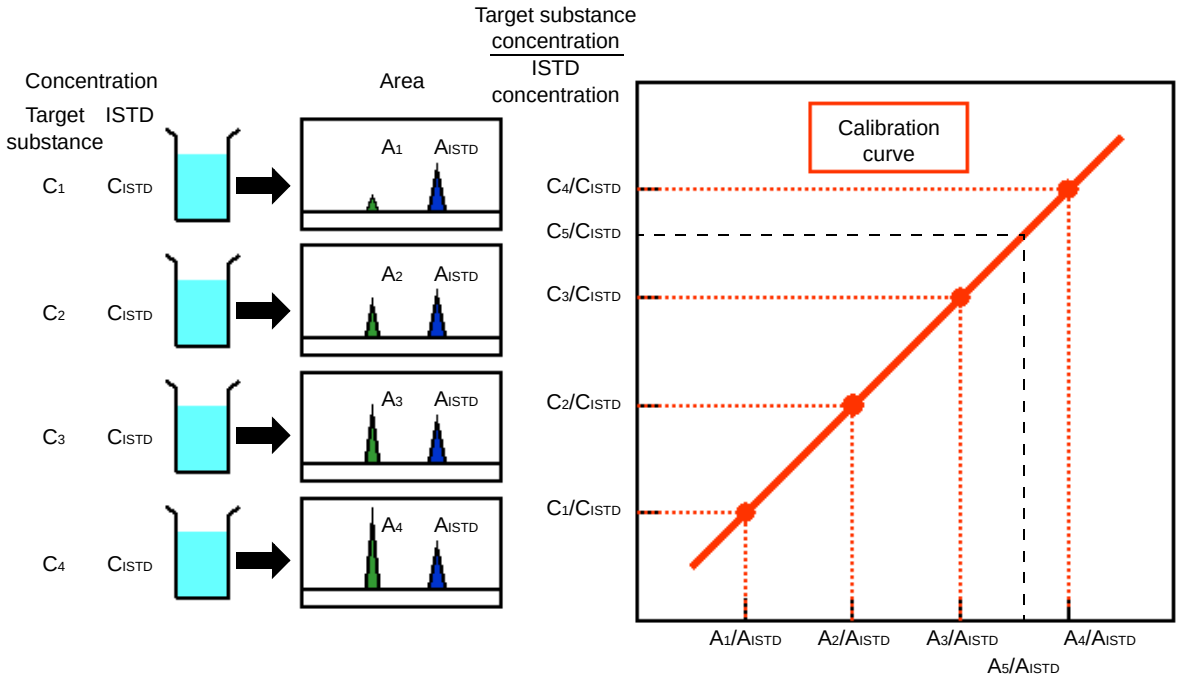



Fig.4-2 Internal Standard Method

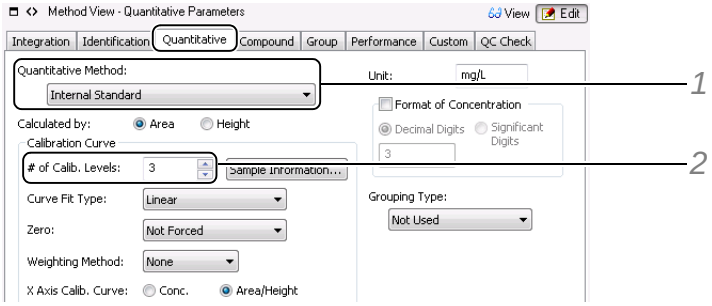
A sample solution is prepared by spiking the unknown sample with the same concentration of ISTD as was used in the standard solution preparation. Data acquisition is performed on the same volume of unknown sample solution under the same conditions used to analyze the standard solutions.

The peak area ratio between X and ISTD (A5/Aistd.) for the unknown sample is calculated and the concentration ratio (C5/Cistd) is calculated from the calibration curve.

This section describes how to quantitate using the “internal standard method”.

**1** **Click Edit (Edit Mode) in [Method View].**

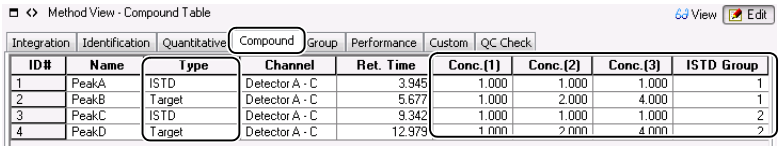
**2** **Click the [Quantitative] tab, and set each parameter.**




1 Select [Internal Standard] for the [Quantitative Method].
2 Enter the number of concentration levels (calibration points) at [# of Calib. Levels].

**3** **Click the [Compound] tab, and set the [Type], [Conc.], and [ISTD Group] for each compound.**

This example uses the following calibration curve parameters.




| ID# | Name | Type | Channel | Ret. Time | Conc.(1) | Conc.(2) | Conc.(3) | ISTD Group |
|---|---|---|---|---|---|---|---|---|
| 1 | PeakA | ISTD | Detector A - C | 3.945 | 1.000 | 1.000 | 1.000 | 1 |
| 2 | PeakB | Target | Detector A - C | 5.677 | 1.000 | 2.000 | 4.000 | 1 |
| 3 | PeakC | ISTD | Detector A - C | 9.342 | 1.000 | 1.000 | 1.000 | 2 |
| 4 | PeakD | Target | Detector A - C | 12.979 | 1.000 | 2.000 | 4.000 | 2 |

Make a calibration curve using 3 concentrations of standard solution:

- Peak A: ISTD
- Peak B: Target substance. Quantitated using Peak A.
- Peak C: ISTD
- Peak D: Target substance. Quantitated using Peak C.

**NOTE**

- The ISTD concentration values are used to calculate the calibration curve as the ISTD amount.
- If multiple ISTDs are used, number the substances in the [ISTD Group] column so that the ISTDs corresponding to the target substance are in the same ISTD group.

**4** **Click View (View Mode) in [Method View].**

**NOTE**

- The amount of ISTD in the standard sample is entered in the Compound Table. The amount of ISTD in unknown samples is entered in the Batch Table and in single run. Refer to *"3.6.2 Edit Batch Tables" P.72* for details on entering the ISTD amount.
- To make a calibration curve with multiple calibration points (levels) add equivalent amounts of ISTD to standard solutions of different concentrations. If the standard solution is spiked with the ISTD before it is diluted, only a 1-point calibration curve is created.
- Prepare standard sample solutions by diluting a stock solution in stages to achieve multiple concentrations of the target substance. Prepare the unknown sample solution at the appropriate concentration. Spike all of the diluted standard samples and the unknown sample with equal amounts of the ISTD.
  When the unknown sample is spiked with the same amount of ISTD as the standard solution, quantitative calculation can be performed by comparing the sample amount and ISTD amount with all levels of the ISTD concentration fields set to “1”.

**5** **Save the method file before creating the calibration curve.**

**Reference**

For details on how to make calibration curves, see *"3 Realtime Batch" P.43* or *"14 LC Calibration Curves" P.391*.

## 4.4.3 Standard Addition Method

This method involves analyzing an unknown sample that has been spiked with a known amount of the target substance and an unspiked unknown sample. Quantitation is performed using the difference between the measured peak areas or heights.

Equivalent aliquots of the same unknown sample solution are prepared. One aliquot remains unspiked and the other aliquots are spiked with differing known concentrations of the target substance. All of the unknown sample solutions are analyzed and the results are used to quantitatively calculate the amount of target substance in the unspiked unknown sample. The calibration curve created with the spiked amount of substance (concentration) as the horizontal axis and peak area or height as the vertical axis.

This method is often used in situations where the components of unknown sample matrix compromise the sensitivity of the target substance.

The sample solution (source solution) is divided into several equal parts, and each part is spiked with standard solution and used for data acquisition.
(Example C1: unspiked, C2: 1.0 mg/L, C3: 2.0 mg/L)

The calibration points of the peak area (A1, A2, A3) and spiked amount (0, 1.0 mg/L, 2.0 mg/L) from the data acquisition results, are used to make a 3-point calibration curve (linear).

The absolute value where the calibration curve intersects the X-axis (point of intersection - C4) indicates the concentration (X) of the target component.

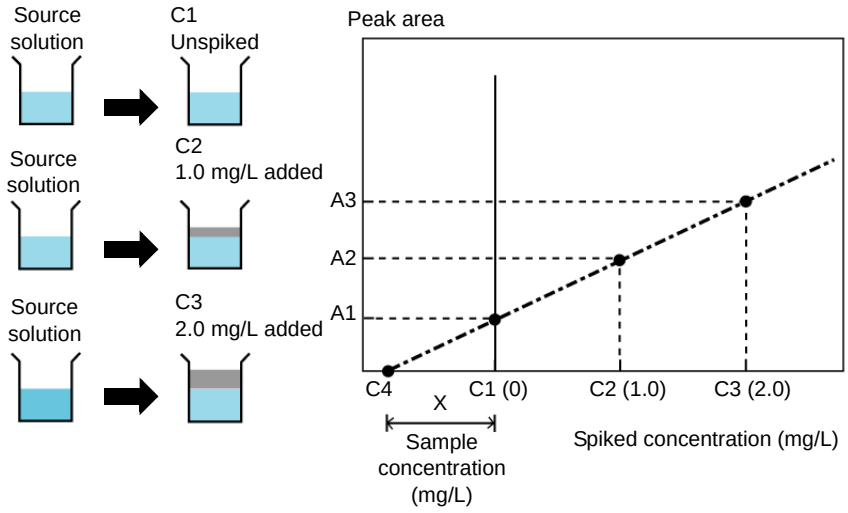
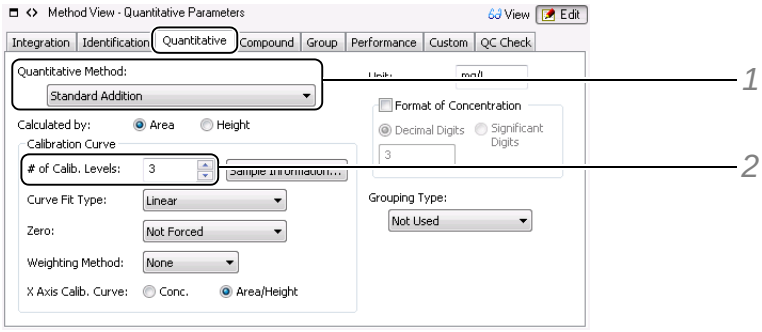



Fig.4-3 Standard Addition Method

This section describes how to quantitate using “standard addition method”.

## 1 Click Edit (Edit Mode) in [Method View].

## 2 Click the [Quantitative] tab, and set each parameter.




1 Select [Standard Addition] for the [Quantitative Method].

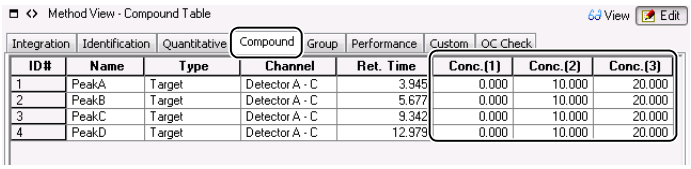
2 Enter the number of concentration levels (calibration points) at [# of Calib. Levels].

**NOTE**

The unspiked sample is one calibration point and 2 spiked samples are used, making the number of calibration points, 3. (1 unspiked sample + 2 spiked samples = 3). Therefore, set the number of levels to “3”.

## 3 Click the [Compound] tab, and enter the [Conc.] of the standard sample.

This example uses the following calibration curve parameters.




| ID# | Name | Type | Channel | Ret. Time | Conc.(1) | Conc.(2) | Conc.(3) |
|---|---|---|---|---|---|---|---|
| 1 | PeakA | Target | Detector A - C | 3.945 | 0.000 | 10.000 | 20.000 |
| 2 | PeakB | Target | Detector A - C | 5.677 | 0.000 | 10.000 | 20.000 |
| 3 | PeakC | Target | Detector A - C | 9.342 | 0.000 | 10.000 | 20.000 |
| 4 | PeakD | Target | Detector A - C | 12.979 | 0.000 | 10.000 | 20.000 |

- Level 1: Unspiked sample “concentration = 0"
- Level 2: 10 mg/L spiked sample
- Level 3: 20 mg/L spiked sample

**NOTE**

- Enter “0” for [Conc. (1)] since it is used for the unspiked sample calibration point.
- Set [Type] to standard for the unspiked and all of the spiked samples, and perform data acquisition using the method file saved above. (Perform postrun batch analysis if the data has already been acquired.)
  Then, change [Type] to [Unknown] for only the unspiked sample, and reprocess the data using the using the method file that contains this calibration curve to obtain the quantitative results.

## 4 Click View (View Mode) in [Method View].

## 4.4.4 Corrected Area Normalization Method

This method involves, first, correcting the peak area or height of each component peak in an unknown sample and totaling these values. The percentage of the corrected area or height for each component with is calculated with respect to that total value is assumed to be the quantitative value.

This section describes how to obtain the sensitivity correction factor using a standard sample of known concentration and how to perform quantitation by the “corrected area normalization” method by manually entering that sensitivity correction factor.

**NOTE**

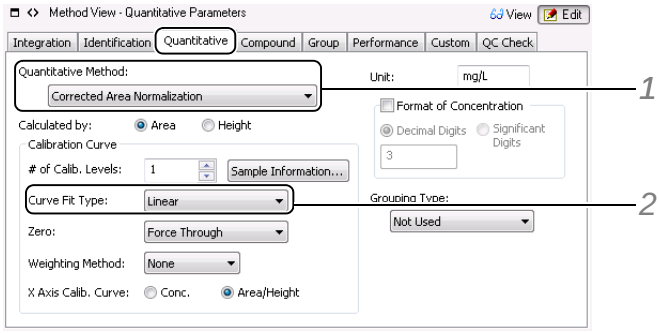
With corrected area normalization, the percentage of the area or height value of all detected peaks is assumed to be the quantitative value.

### ■ Sensitivity Correction Factor Using a Standard Sample

This section describes use of a mixed sample as the standard sample.

**1** **Click Edit (Edit Mode) in [Method View].**

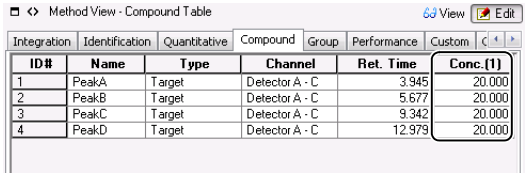
**2** **Click the [Quantitative] tab, and set each parameter.**




*1* Select [Corrected Area Normalization] for the [Quantitative Method].

*2* Select [Linear] for the [Curve Fit Type].

**3** **Enter the concentration in the [Conc.(1)] cell for each compound in the [Compound] tab.**




| ID# | Name | Type | Channel | Ret. Time | Conc.(1) |
|---|---|---|---|---|---|
| 1 | PeakA | Target | Detector A - C | 3.945 | 20.000 |
| 2 | PeakB | Target | Detector A - C | 5.677 | 20.000 |
| 3 | PeakC | Target | Detector A - C | 9.342 | 20.000 |
| 4 | PeakD | Target | Detector A - C | 12.979 | 20.000 |

**4** **Click View (View Mode) in [Method View].**

**NOTE**

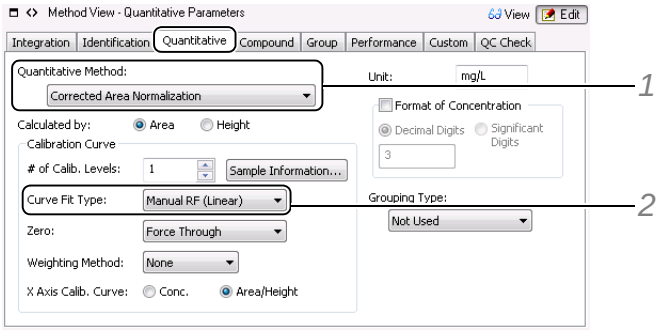
Refer to *"14.1 Calibration Curves by Postrun Batch"* and use the standard sample data to make a calibration curve. The 1st coefficient obtained is the sensitivity correction factor.

## ■ Enter the Sensitivity Correction Factor

This section describes how to manually enter the sensitivity correction factor if it is known.

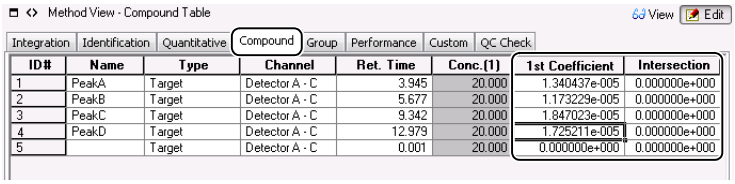
**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Quantitative] tab, and set each parameter.**




*1* Select [Corrected Area Normalization] for the [Quantitative Method].
*2* Select [Manual RF (Linear)] for the [Curve Fit Type].

**3** **Enter the sensitivity correction factor in the [1st Coefficient] cell for each compound in the [Compound] tab.**




| ID# | Name | Type | Channel | Ret. Time | Conc.(1) | 1st Coefficient | Intersection |
|---|---|---|---|---|---|---|---|
| 1 | PeakA | Target | Detector A - C | 3.945 | 20.000 | 1.340437e-005 | 0.000000e+000 |
| 2 | PeakB | Target | Detector A - C | 5.677 | 20.000 | 1.173229e-005 | 0.000000e+000 |
| 3 | PeakC | Target | Detector A - C | 9.342 | 20.000 | 1.847023e-005 | 0.000000e+000 |
| 4 | PeakD | Target | Detector A - C | 12.979 | 20.000 | 1.725211e-005 | 0.000000e+000 |
| 5 | | Target | Detector A - C | 0.001 | 20.000 | 0.000000e+000 | 0.000000e+000 |

**4** **Click View (View Mode) in [Method View].**

## 4.4.5 Grouping

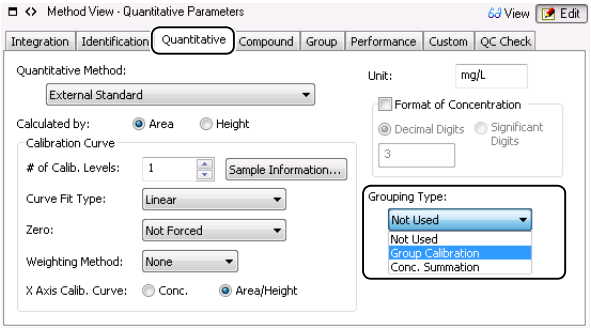
Bundling homologs or isomers when there are multiple compounds is called “grouping”.

Grouping is effective in dividing the peaks into groups to perform quantitative analysis only on individual groups or when measuring the amount of impurities in a certain main component as a single group.

This section describes how to perform grouping quantitation.

**1** **Click Edit (Edit Mode) in [Method View].**

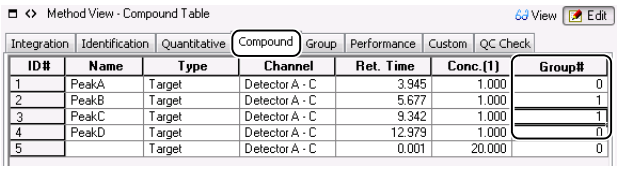
**2** **Click the [Quantitative] tab, and select [Group Calibration] or [Conc. Summation] for the [Grouping Type].**




**NOTE**

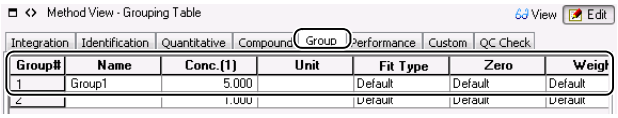
- The sum of the peak areas or heights of the grouped compounds is used with [Group Calibration], a calibration curve is created for each group, and quantitation is performed for each group.
- A calibration curve is created for each compound and quantitation is performed for each compound, with [Conc. Summation]. Then the sum of the concentrations of the grouped compounds is used as the concentration of the group.

**3** **Click the [Compound] tab, and enter the same group number in the [Group#] column of all of the compounds in a group.**




| ID# | Name | Type | Channel | Ret. Time | Conc.(1) | Group# |
|---|---|---|---|---|---|---|
| 1 | PeakA | Target | Detector A - C | 3.945 | 1.000 | 0 |
| 2 | PeakB | Target | Detector A - C | 5.677 | 1.000 | 1 |
| 3 | PeakC | Target | Detector A - C | 9.342 | 1.000 | 1 |
| 4 | PeakD | Target | Detector A - C | 12.979 | 1.000 | 0 |
| 5 | | Target | Detector A - C | 0.001 | 20.000 | 0 |

**4** **Click the [Group] tab, and enter [Name], [Conc.], and [Unit].**




| Group# | Name | Conc.(1) | Unit | Fit Type | Zero | Weigh |
|---|---|---|---|---|---|---|
| 1 | Group1 | 5.000 | | Default | Default | Default |

**5** **Click View (View Mode) in [Method View].**

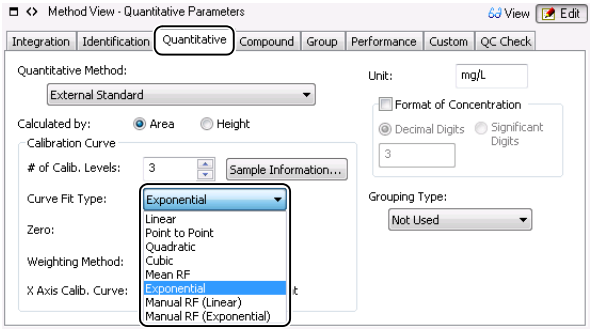
## 4.4.6 Calibration Curve for Exponential Calculation

Since the sample concentration and sensitivity are not directly proportional when using an LC-ELSD detector, make a calibration curve using the exponential function.

This section describes how to perform quantitative calculation using a calibration curve calculated from the exponential function.

**1** **Click Edit (Edit Mode) in [Method View].**

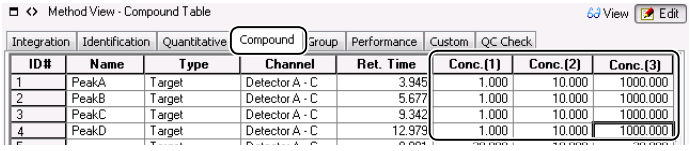
**2** **Click the [Quantitative] tab, and select [Exponential] for the [Curve Fit Type].**




**NOTE**

- At least 2 standard samples (i.e. 2 calibration points) are required to create a calibration curve with the exponential calculation. Select 2 or higher at [# of Calb. Levels].
- [Zero] cannot be set for the exponential calibration curve since the curve does not pass through the origin.
- Both of the axes of the graph for the exponential calibration curve are logarithmic.

**3** **Click the [Compound] tab, and enter the [Conc.](s).**




**4** **Click View (View Mode) in [Method View].**

## 4.4.7 Standard Concentration Factor

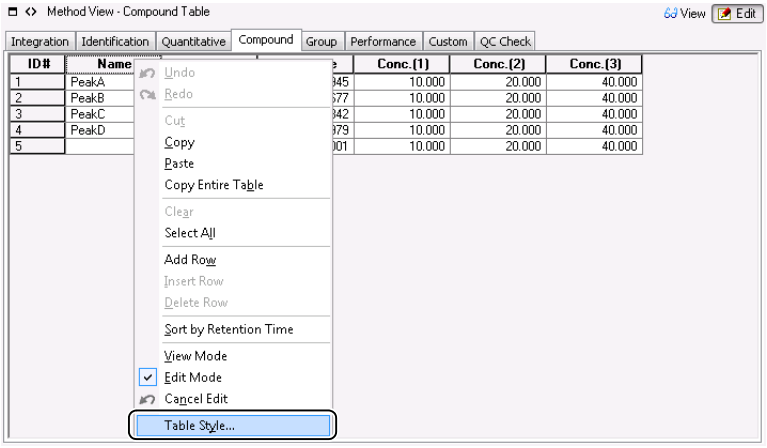
Make a calibration curve using values obtained by multiplying concentration values of each level with compensation factors.

This section describes how to set the standard concentration factor.

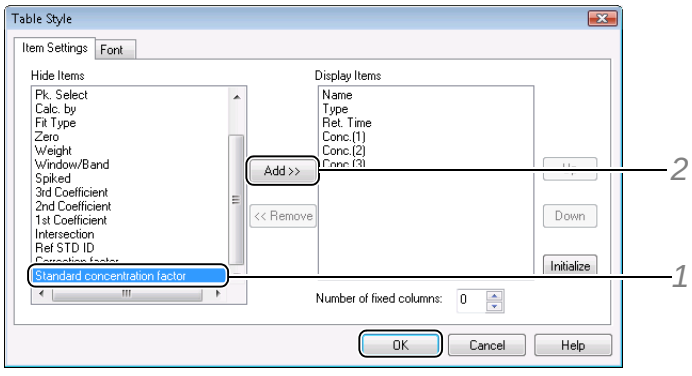
**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Compound] tab.**

**3** **Right-click on the Compound Table, and click [Table Style].**




**4** **Add the [Standard concentration factor] column to the Compound Table in the [Table Style] sub-window, and click [OK].**




*1* Select [Standard concentration factor] in the [Hide Items] list.

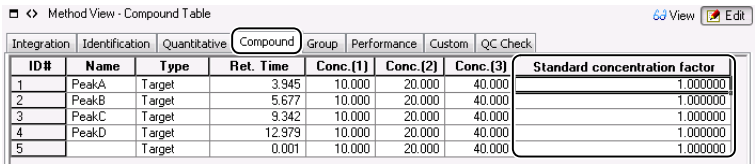
*2* Click [Add].

The [Standard concentration factor] item is added to [Display Items] list.

**NOTE**

Change the display order of items in the Compound Table, by selecting the item in the [Display Items] list and then clicking [Up] or [Down].

**5** **Enter the [Standard concentration factor] column.**




| ID# | Name | Type | Ret. Time | Conc.(1) | Conc.(2) | Conc.(3) | Standard concentration factor |
|---|---|---|---|---|---|---|---|
| 1 | PeakA | Target | 3.945 | 10.000 | 20.000 | 40.000 | 1.000000 |
| 2 | PeakB | Target | 5.677 | 10.000 | 20.000 | 40.000 | 1.000000 |
| 3 | PeakC | Target | 9.342 | 10.000 | 20.000 | 40.000 | 1.000000 |
| 4 | PeakD | Target | 12.979 | 10.000 | 20.000 | 40.000 | 1.000000 |
| 5 | | Target | 0.001 | 10.000 | 20.000 | 40.000 | 1.000000 |

**6** **Click View (View Mode) in [Method View].**

## 4.4.8 Reference Standard ID and Correction Factor

If standards cannot be prepared for impurities or related substances, create a calibration curve using a standard substance with the same (or proportional) response factor, and quantitate the concentration of the impurities or related substances using that calibration curve.

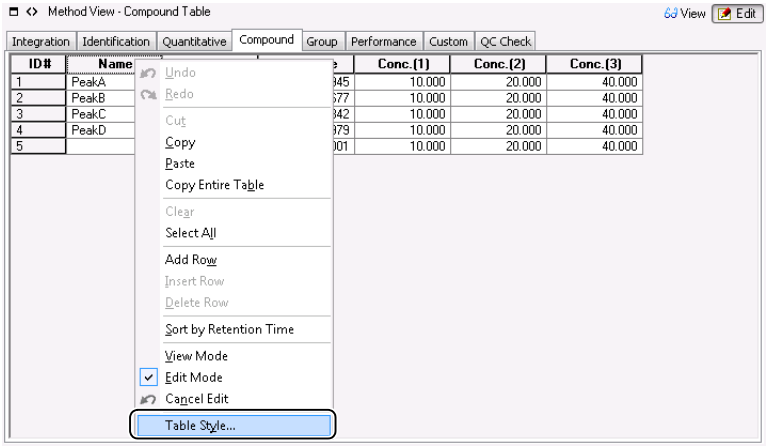
**NOTE**

Use the value obtained by multiplying the peak area or height or the peak area or height ratio of the internal standard by the correction factor, to create the reference standard calibration curve specified by ID.

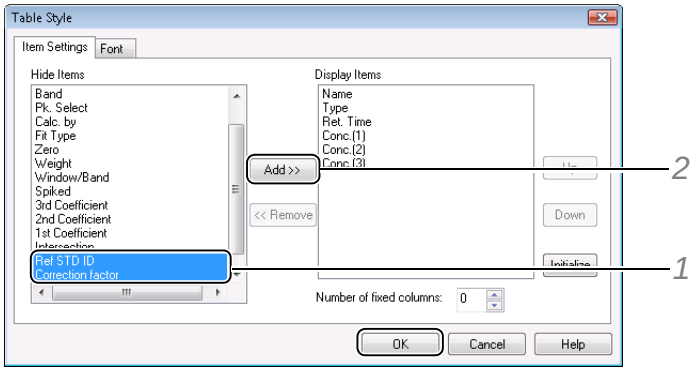
**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Compound] tab.**

**3** **Right-click on the Compound Table, and click [Table Style].**



## 4 Add the [Ref STD ID] and the [Correction factor] column to the Compound Table in the [Table Style] sub-window, and click [OK].




1 Select [Ref STD ID] and [Correction factor] in the [Hide Items] list.

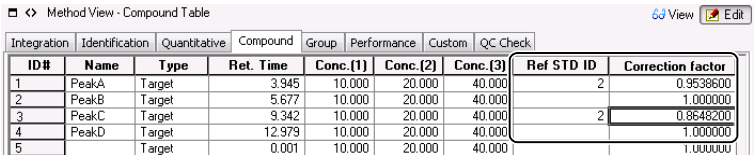
2 Click [Add].

The [Ref STD ID] and [Correction factor] item are added to the [Display Items] list.

**NOTE**

Change the display order of items in the Compound Table, by selecting the item in the [Display Items] list and then clicking [Up] or [Down].

## 5 Enter the [Ref STD ID] and [Correction factor] column.




| ID# | Name | Type | Ret. Time | Conc.(1) | Conc.(2) | Conc.(3) | Ref STD ID | Correction factor |
|---|---|---|---|---|---|---|---|---|
| 1 | PeakA | Target | 3.945 | 10.000 | 20.000 | 40.000 | 2 | 0.9538600 |
| 2 | PeakB | Target | 5.677 | 10.000 | 20.000 | 40.000 | | 1.000000 |
| 3 | PeakC | Target | 9.342 | 10.000 | 20.000 | 40.000 | 2 | 0.8648200 |
| 4 | PeakD | Target | 12.979 | 10.000 | 20.000 | 40.000 | | 1.000000 |
| 5 | | Target | 0.001 | 10.000 | 20.000 | 40.000 | | 1.000000 |

## 6 Click View (View Mode) in [Method View].

# 4.5 Compound Table

The Compound Table must be completed to identify detected peaks or to perform quantitative calculation on the detected peaks. There are various ways of entering data into the Compound Table. Use the method that is the most convenient.

- *"Compound Table Wizard"*
- *"Compound Table from the Peak Table"*
- *"Compound Table Retention Times Using the Mouse"*
- *"Directly Edit the Compound Table"*

## 4.5.1 Compound Table Wizard

This section describes how to complete a Compound Table using the wizard. Using the wizard also allows the peak integration, peak identification, and quantitative parameters to be entered in the consecutive sub-windows.

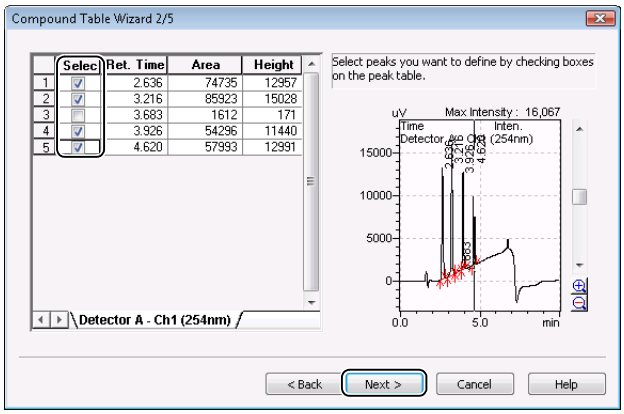
**1** **Click the (Wizard) icon on the [Data Analysis] assistant bar.**

**2** **Enter the peak integration parameters, and click [Next].**

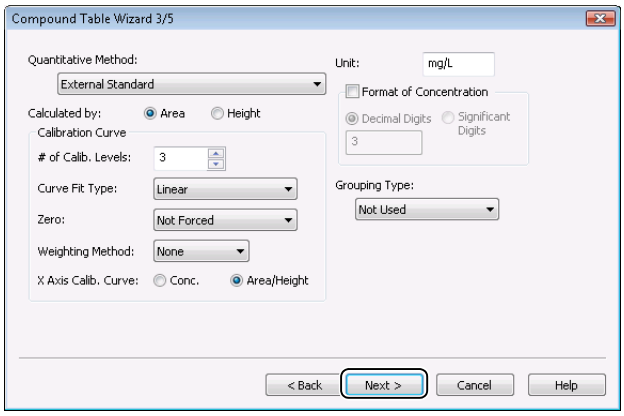
**Reference**

Refer to *"4.2 Peak Integration Parameters" P.88* for details on setting the peak integration parameters.

**3** **Select the [Select] column to register a peak in the Compound Table, and click [Next].**




**4** **Enter the quantitative parameters, and click [Next].**




**Reference**

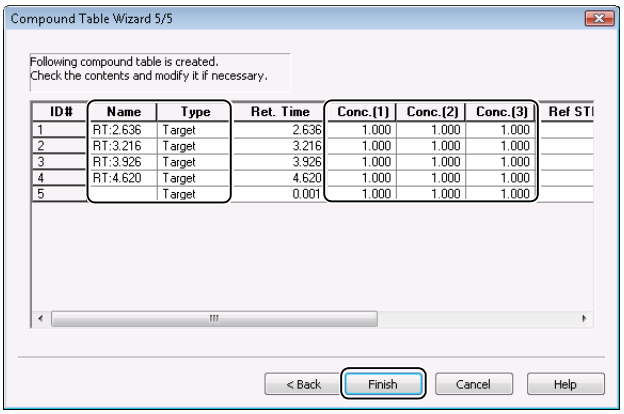
Refer to *"4.4 Quantitative Parameters" P.103* for details on setting the quantitative parameters.

**5** **Enter the peak identification parameters, and click [Next].**

**Reference**

Refer to *"4.3 Peak Identification Parameters" P.101* for details on setting the peak identification parameters.

**6** **Enter the [Name], [Type] and [Conc.] column in the Compound Table, and click [Finish].**




**NOTE**

- The default [Name] is “RT (Retention Time) + peak retention time”.
- Edit the Compound Table to match the parameters set in quantitative processing.

The settings made in the wizard are saved to the data processing parameters in the open data file.

**Reference**

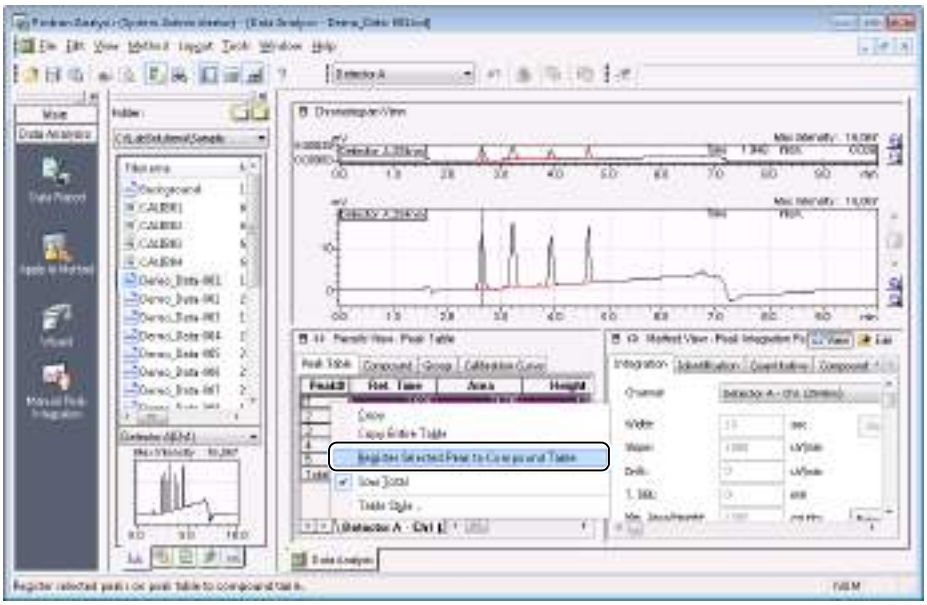
- Refer to *"4.7 Save (Export) to Method Files" P.126* to save settings made in the wizard to method file.
- Refer to *"14 LC Calibration Curves" P.391* for details on creating calibration curves.

## 4.5.2 Compound Table from the Peak Table

Peaks displayed in [Chromatogram View] can be registered to the [Compound] tab in [Method View]. This section describes how to register peaks in [Chromatogram View] to the Compound Table.

**1** **Click the [Peak Table] tab in [Results View].**

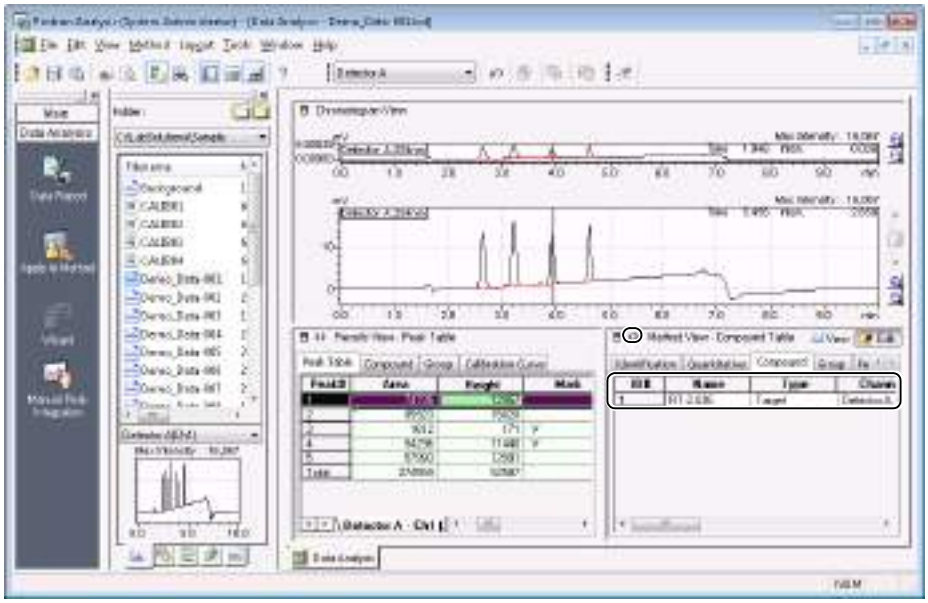
**2** **Right-click [Peak#] for the desired peak, and click [Register Selected Peak to Compound Table].**



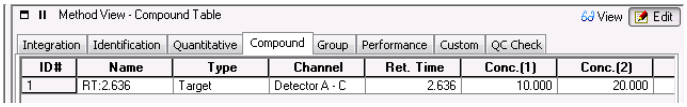
The selected peaks in the Peak Table are registered to the Compound Table.

**3** **Click the [Compound] tab in [Method View].**

**4** **Enter [Name] and [Conc.] of the registered peak in the Compound Table.**



Click the <> (Wide Size) button to maximize the view width. Click the || (Normal Size) button to restore the view size.




**5** **Click View (View Mode) in [Method View].**

### Reference

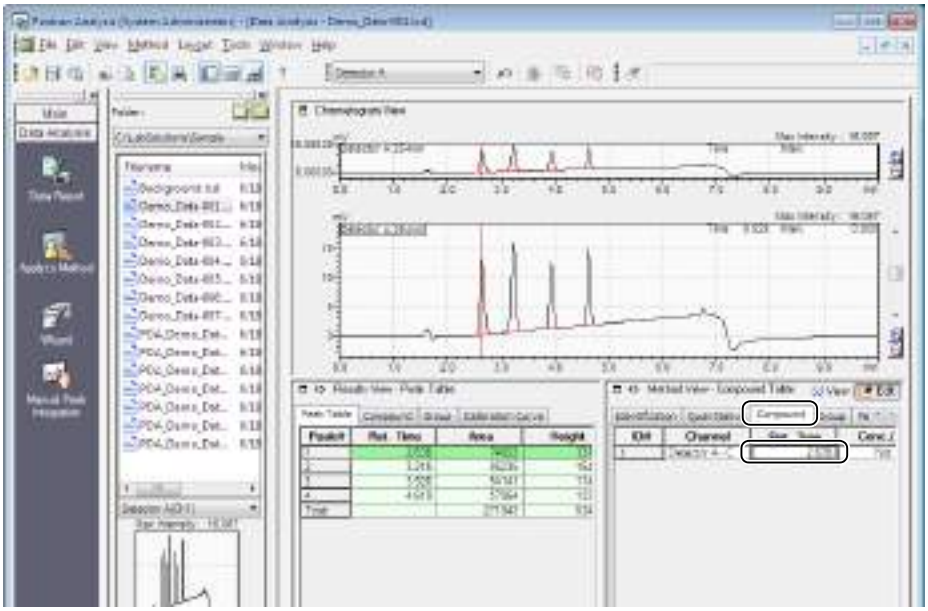
- Refer to *"4.7 Save (Export) to Method Files" P.126* for details on saving to the method file.
- Refer to *"14 LC Calibration Curves" P.391* For details on creating calibration curves.

## 4.5.3 Compound Table Retention Times Using the Mouse

Retention times in the Compound Table can be easily set with the mouse in [Chromatogram View].

**1** **Click** Edit **(Edit Mode) in [Method View].**

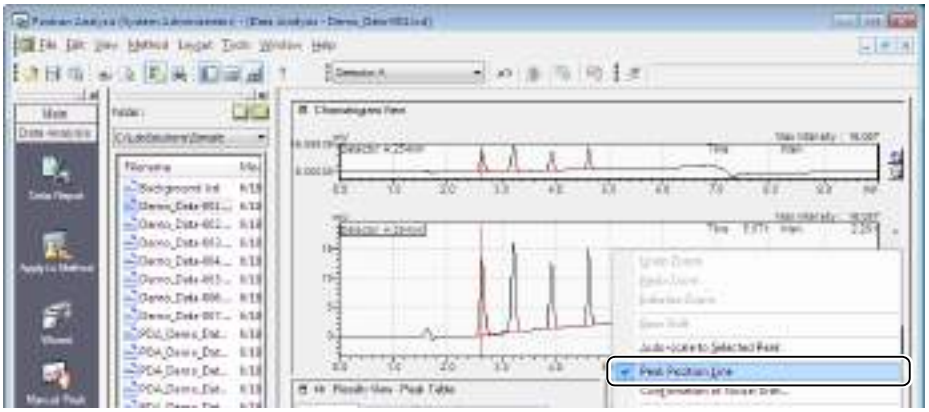
**2** **Click the [Compound] tab, and select the desired [Ret. Time] cell.**



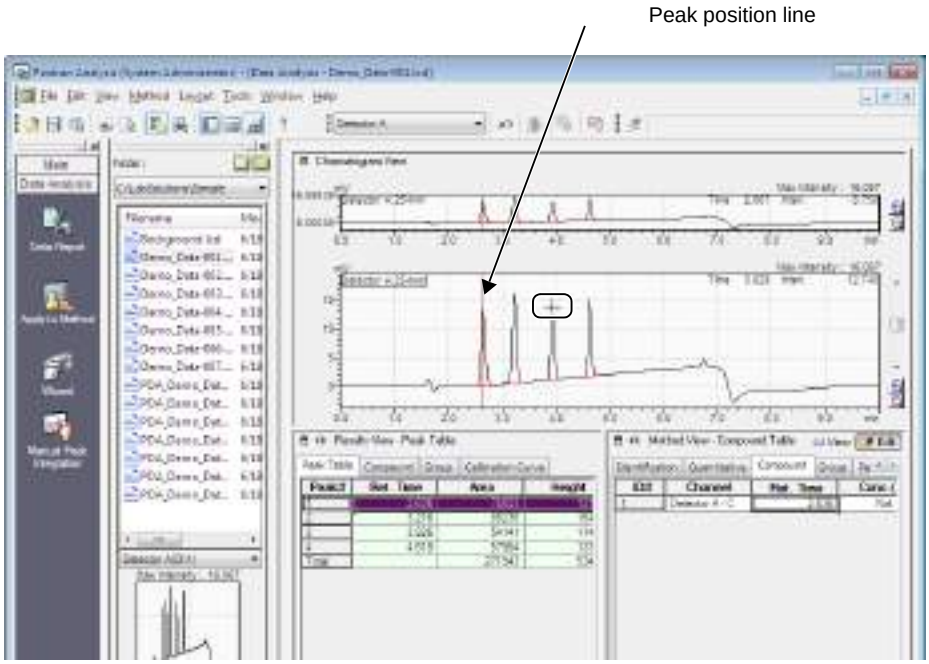
The peak position lines are displayed in red in the [Chromatogram View].

**NOTE**

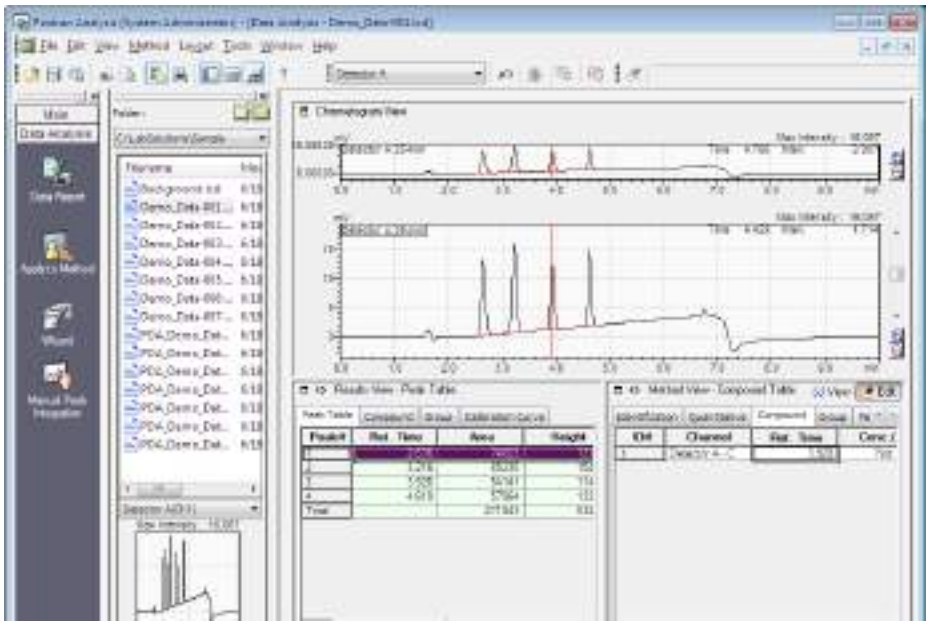
Right-click on the chromatogram, and if [Peak Position Line] on the displayed menu is not selected, select [Peak Position Line] to display the peak position line.



## 3 Select the peak whose retention time is to be changed.




The retention time change is automatically registered to the Compound Table.



**NOTE**

Fine-adjust the peak position line by dragging the line with the [Shift] key held down.

## 4 Click View (View Mode) in [Method View].

### Reference

- Refer to *"4.7 Save (Export) to Method Files" P.126* for details on saving to the method file.
- Refer to *"14 LC Calibration Curves" P.391* for details on creating calibration curves.

## 4.5.4 Directly Edit the Compound Table

Click the target compound cell to edit a cell in the Compound Table.

This section describes how to select the Window/Band method and compound type.

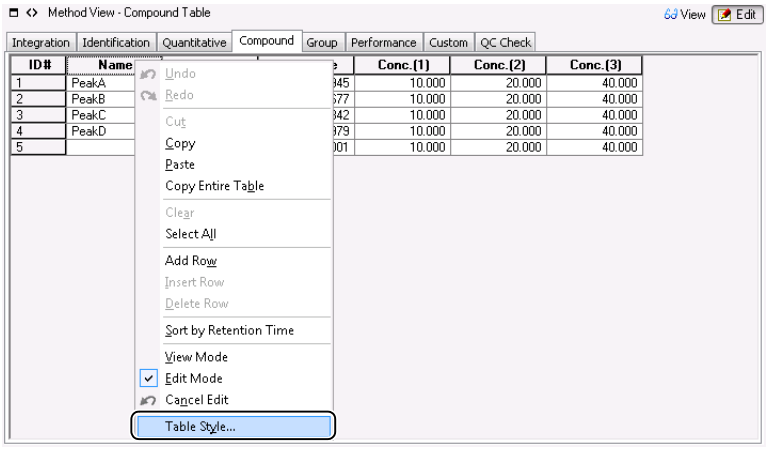
### ■ Select the Window/Band Method for Each Compound

The identification method set on the [Identification] tab in [Method View] is used for all of the compounds. It can also be set to each compound in the Compound Table.

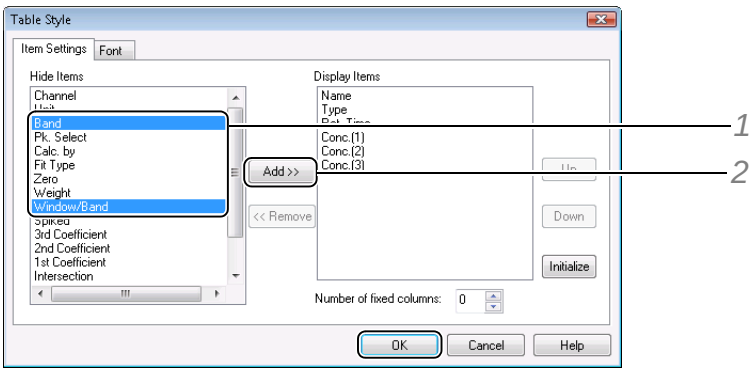
**1** **Click [Edit] (Edit Mode) in [Method View].**

**2** **Click the [Compound] tab.**

**3** **Right-click on the Compound Table, and click [Table Style].**




**4** **Add the [Window/Band] and the [Band] column to the Compound Table in the [Table Style] sub-window, and click [OK].**




*1* Select [Window/Band] and [Band] in the [Hide Items] list.

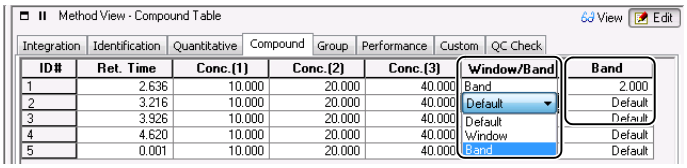
*2* Click [Add].

The [Window/Band] and [Band] item are added to the [Display Items] list.

**NOTE**

Change the display order of items in the Compound Table, by selecting the item in the [Display Items] list and then clicking [Up] or [Down].

**5** **Set [Window/Band] and [Band] parameters.**




1 Click the [Window/Band] cell for the desired compound, and select [Default], [Window] or [Band].
2 Enter the allowable time width in the [Band] cell, if [Band] is selected.

**NOTE**
If [Window/Band] is set to [Default], the value set on the [Identification] tab is used.

**6** **Click View (View Mode) in [Method View].**

**Reference**

- Refer to *"4.7 Save (Export) to Method Files" P.126* for details on saving to the method file.
- Refer to *"14 LC Calibration Curves" P.391* for details on creating calibration curves.

## ■ Compound Type

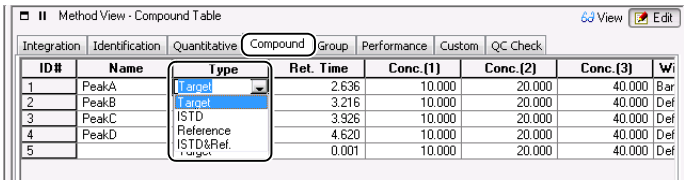
This section describes how to set the reference compound for peak identification using the relative retention time method.

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Compound] tab, and select the [Type].**

Click the [Type] cell of the desired compound, and select [Reference].

**NOTE**
Use this method to set the ISTD as the reference for the internal standard method. Click the [Type] cell of the ISTD, and select [ISTD & Ref.].




**3** **Click View (View Mode) in [Method View].**

**NOTE**
If changes are made to the parameters such as [Type] on the [Compound] tab, the calibration curve will change. In this case, the current calibration curve information saved in the data file is automatically deleted.

**Reference**

- Refer to *"4.7 Save (Export) to Method Files" P.126* for details on saving to the method file.
- Refer to *"14 LC Calibration Curves" P.391* for details on creating calibration curves.

# 4.6 Column Performance Parameters

This section describes how to set the various calculation methods for supporting the system suitability test and how to check calculation results.

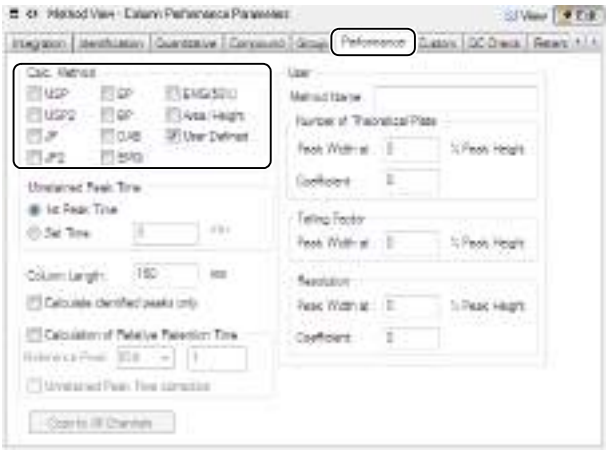
- USP
- USP2
- JP
- JP2
- EP
- BP
- DAB
- EMG
- EMG (50%)
- area/height
- user-defined

**Reference**

For details about the column performance equations, refer to Help or the Data Acquisition & Processing Theory Guide.

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Performance] tab, and select the appropriate checkbox(es) at [Calc. Method].**

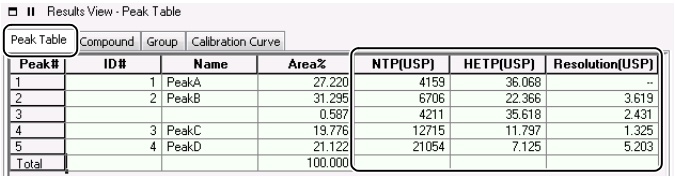


**NOTE**

- Select [User Defined] to display the [User] parameters box.
- Either select [1st Peak Time] or enter a [Set Time] at [Unretained Peak Time].
- Select [Column Length] to calculate the number of theoretical plates.

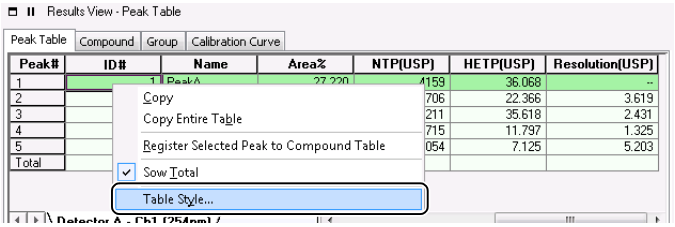
**3** **Click View (View Mode) in [Method View].**

**4** **Click the [Peak Table] tab in [Results View], and check the number of theoretical plates and resolution.**

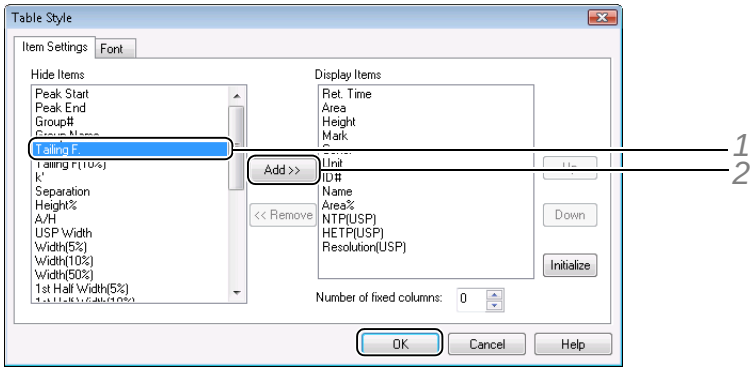



| Peak# | ID# | Name | Area% | NTP(USP) | HETP(USP) | Resolution(USP) |
|---|---|---|---|---|---|---|
| 1 | 1 | PeakA | 27.220 | 4159 | 36.068 | -- |
| 2 | 2 | PeakB | 31.295 | 6706 | 22.366 | 3.619 |
| 3 | | | 0.587 | 4211 | 35.618 | 2.431 |
| 4 | 3 | PeakC | 19.776 | 12715 | 11.797 | 1.325 |
| 5 | 4 | PeakD | 21.122 | 21054 | 7.125 | 5.203 |
| Total | | | 100.000 | | | |

**5** **To check the tailing factor, right-click on the Peak Table, and click [Table Style].**




**6** **Add the [Tailing F.] column to the Compound Table in the [Table Style] sub-window, and click [OK].**




*1* Select [Tailing F.] in the [Hide Items] list.

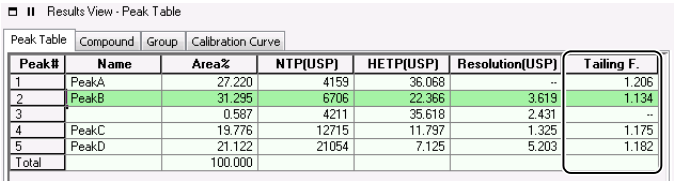
*2* Click [Add].

The [Tailing F.] item is added to the [Display Items] list.

**NOTE**

Change the display order of items in the Compound Table, by selecting the item in the [Display Items] list and then clicking [Up] or [Down].

[Tailing F.] is displayed in the Peak Table.




| Peak# | Name | Area% | NTP(USP) | HETP(USP) | Resolution(USP) | Tailing F. |
|---|---|---|---|---|---|---|
| 1 | PeakA | 27.220 | 4159 | 36.068 | -- | 1.206 |
| 2 | PeakB | 31.295 | 6706 | 22.366 | 3.619 | 1.134 |
| 3 | | 0.587 | 4211 | 35.618 | 2.431 | -- |
| 4 | PeakC | 19.776 | 12715 | 11.797 | 1.325 | 1.175 |
| 5 | PeakD | 21.122 | 21054 | 7.125 | 5.203 | 1.182 |
| Total | | 100.000 | | | | |

**NOTE**

Add [Tailing Factor] or [Resolution] display settings to the [Quantitative Results] report items to print the results in the output report.

# 4.7 Save (Export) to Method Files

After setting the quantitative parameters and the Compound Table, save (export) the new settings to the method file.

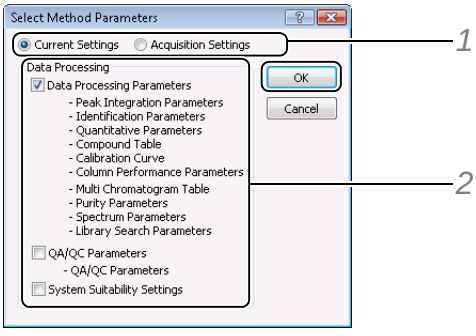
**1** **Click the (Apply to Method) icon on the [Data Analysis] assistant bar.**

**2** **The name of the method file used for data acquisition is displayed. Click [Save].**

**NOTE**

Enter a new name at [File name] to create a new method file.

**3** **Select the method items to save, and click [OK].**




*1* Select [Current Settings].

[Current Settings] saves the latest currently displayed method parameters.
[Acquisition Settings] saves the method parameters used for data acquisition.

*2* Select the method items to save.

The selected method items are saved to the method file.

# 5 PDA Data Analysis

This chapter describes how to analyze chromatograms or spectra obtained by data acquisition with the PDA (photodiode array) detector, execute purity calculations on detected peaks, and perform library searches.

## 5.1 [PDA Data Analysis] Window

The [PDA Data Analysis] window is comprised of the following views:

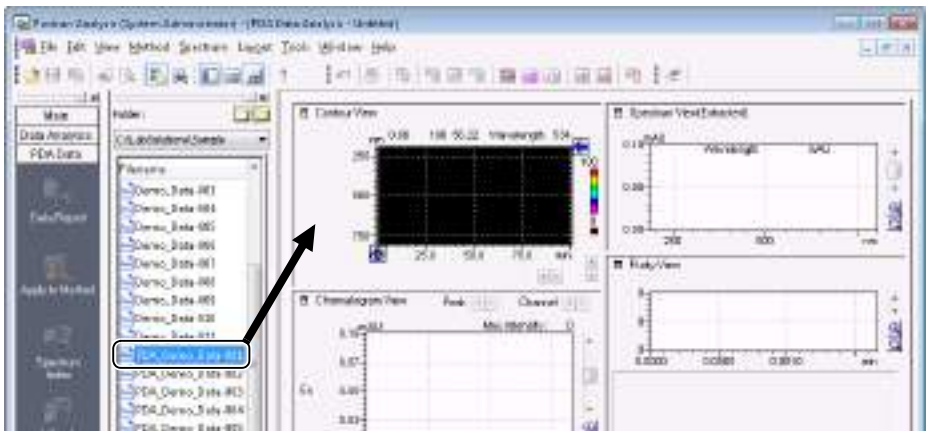
- [Contour View] - displays a contour view with absorbance color-coded
- [Chromatogram View] - displays chromatograms and status curves
- [Spectrum View] - displays the UV spectra
- [Purity View] - displays the purity calculation results of detected peaks
- [Results View] - displays quantitative calculation results
- [Method View] - displays and editing data processing parameters



### 5.1.1 Open the [PDA Data Analysis] Window

**1** **Click the (PDA Data Analysis) icon on the [Main] assistant bar in the [Postrun Analysis] program.**

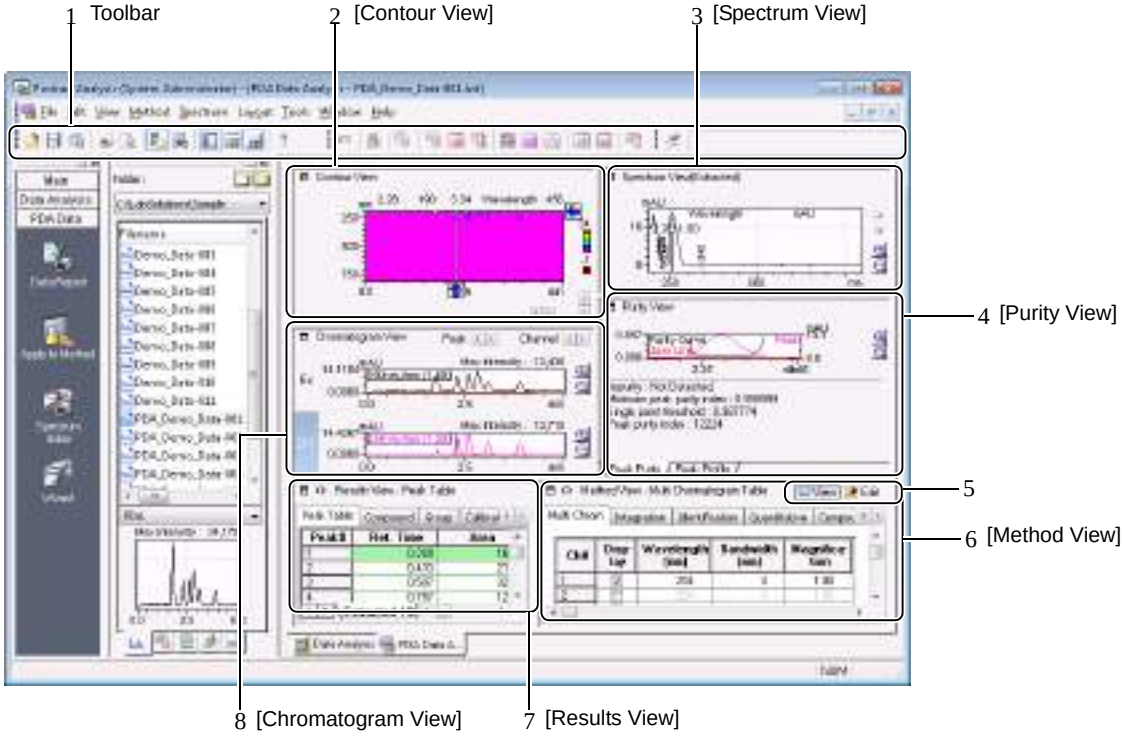
**2** **Drag-and-drop the data file onto the [PDA Data Analysis] window from the [Data Explorer] sub-window.**



The contents of the data file is displayed in the [PDA Data Analysis] window.

## 5.1.2 [PDA Data Analysis] Window Description

This section describes how to view and use the [PDA Data Analysis] window.




| No. | Explanation |
|---|---|
| 1 | Displays the [Standard] and [PDA Data Analysis] toolbars. |
| 2 | Displays the contour graph with PDA data color-coded into absorbance ranges.<br>Drag the and to display the chromatograms and spectra extracted at that position in [Chromatogram View] and [Spectrum View]. |
| 3 | Displays the UV spectrum at selected retention time or a selected peak.<br>Right-click the [Spectrum View] to select operations such as switching of the view mode (Extracted or Registered) and UV library search for selected spectra. |
| 4 | The [Peak Purity] tab displays the purity result for the selected peak.<br>The [Peak Profile] tab displays the overlaid chromatogram for the selected peak at multiple wavelengths. |
| 5 | Select the [Edit] mode to change various parameters in [Method View]. |
| 6 | Displays the data processing parameters of the currently open data file.<br>The [Multi Chrom], [UV Spectrum], [Library Search], and [Purity] tabs are displayed in addition to the tabs displayed in the [Data Analysis] window. |
| 7 | Displays the peak integration and quantitative results.<br>The display content is the same as [Results View] in the [Data Analysis] window. |
| 8 | Displays the chromatogram at the wavelength on the [Multi Chrom] tab in the data processing parameters and the chromatogram extracted from the contour.<br>Right-click on the graph in [Chromatogram View] to select operations such as switching the view mode (Overlay Chromatograms, Stack Chromatograms and Single Chromatogram), registration of multi chromatograms, and manual peak integration.<br>Use to change the channel and peak position. |

**NOTE**

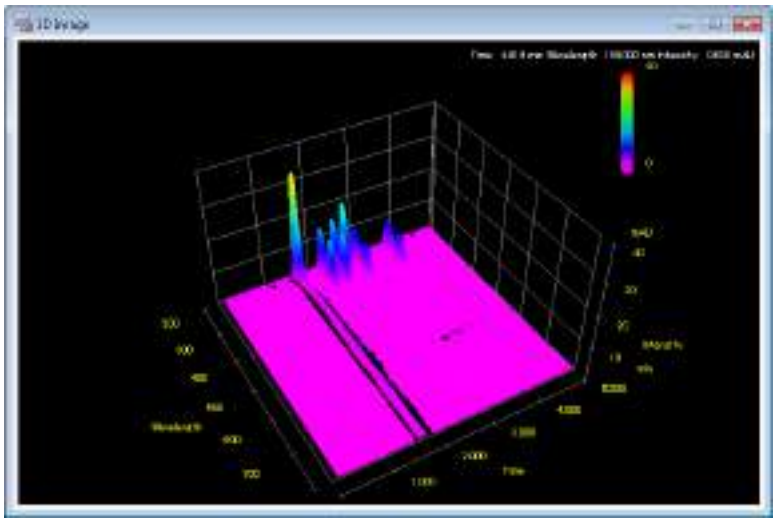
- Only data file can be displayed in the [PDA Data Analysis] window.
  Drag-and-drop the other data files onto the [PDA Data Analysis] window to change to the content of their data files.
- If the data file was acquired by simultaneous use of another detector, the chromatogram acquired by that detector is also displayed in the [Data Analysis] window.

## ■ View the Data in Its Entirety (3D Image)

PDA data can be shown in its entirely as a 3D image.

**1** **Click [3D Image] on the [View] menu.**

The [3D Image] sub-window opens.



**NOTE**

- Click  in the top right corner of the sub-window to close the [3D Image] sub-window.
- The [3D Image] sub-window can be enlarged by dragging on the sub-window, and the display angle can be changed by dragging on the periphery of the 3D display area.
- The [3D Image] sub-window does not support the [256 Colors] Windows graphic mode. Use it in environments with the [High Color] setting or above. Do not change the number of colors for graphics while the [3D Image] sub-window is displayed.

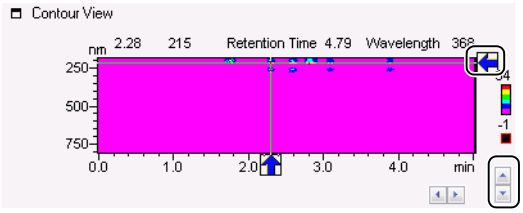
## 5.1.3 Display Chromatograms Extracted from [Contour View]

In [Contour View], the chromatograms or spectra can be extracted from [Contour View] by using the extraction lines.

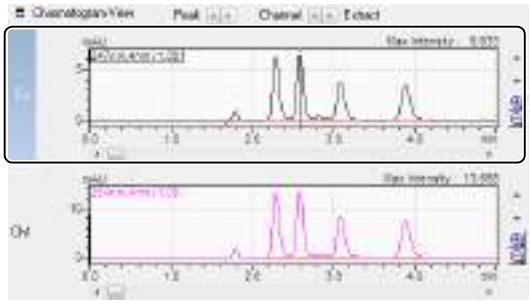
This section describes how to change the extraction position of the wavelength (Y-axis) and display the chromatogram at that position in the [Chromatogram View].

**1** **Drag to move to the target position.**

(Click to fine-adjust the wavelength extraction position.)

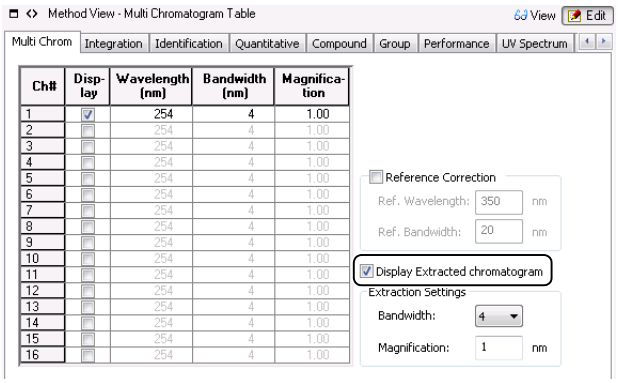



The extracted chromatogram is displayed in the [Ex] (extracted chromatogram) region in the [Chromatogram View].



**NOTE**

- The wavelength extraction position can be checked by the wavelength displayed by on [Contour View] or by the wavelength displayed in the [Ex] region in [Chromatogram View].
- Right-click on [Contour View] and select [Graph Properties] to adjust the Contour Properties. Select [Display Settings] to adjust the Contour View Display Settings.
- The extracted chromatogram is only displayed if [Display Extracted chromatogram] is selected on the [Multi Chrom] tab in [Method View].



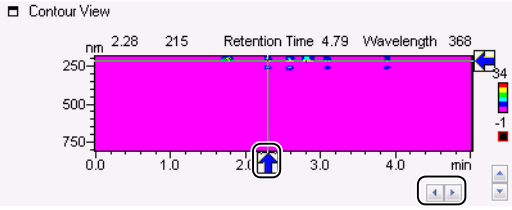
## 5.1.4 Display Spectra Extracted from [Contour View]

The chromatograms or spectra can be extracted from [Contour View] by using the extraction line.

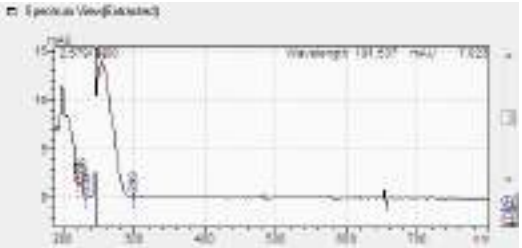
This section describes how to change the extraction position of the time (X-axis) and display the spectrum at that position in the [Spectrum View].

**1** **Drag to move to the target position.**

(Click to fine-adjust the time extraction position. )




The extracted spectrum is displayed in [Spectrum View].



**NOTE**

- The wavelength extraction position can be checked by the wavelength displayed by on [Contour View] or by the retention time displayed in [Spectrum View].
- Right-click on [Contour View] and select [Graph Properties] to adjust the Contour Properties. Select [Display Settings] to adjust the Contour View Display Settings.
- Right-click on the spectrum and select or deselect [Registered Spectrum] and switch between [Spectrum View (Registered)] and [Spectrum View (Extracted)].

## 5.1.5 Manipulate Extracted Chromatograms and Spectra

Double-click anywhere on a chromatogram (or spectrum) display to check the chromatogram waveform or spectrum shape.

### ■ Display the Spectrum of a Desired Retention Time Extracted from the Chromatogram

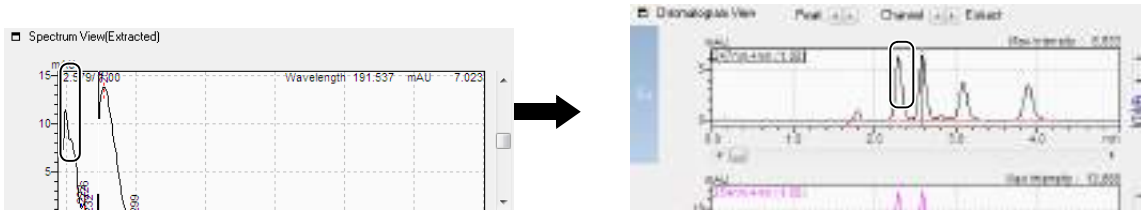
Double-click a selected chromatogram at a desired retention time to display the spectrum of that retention time in [Spectrum View].


**NOTE**

To check the spectrum of a time at the top of a detected peak, click [Peak ]. The spectrum moves to the top of the detected peak.

### ■ Display the Chromatogram of a Desired Wavelength Extracted from the Spectrum

Double-click a desired wavelength of a spectrum to display the chromatogram at that wavelength in the [Ex] (extracted chromatogram] section of the [Chromatogram View].




**NOTE**

- Chromatograms extracted from [Spectrum View] cannot be displayed if a channel other than [Ex] (extracted chromatogram) is selected in [Chromatogram View].
- The extracted chromatogram cannot be displayed if [Display Extracted chromatogram] is deselected on the [Multi Chrom] tab in [Method View].

# 5.2 Register Chromatograms

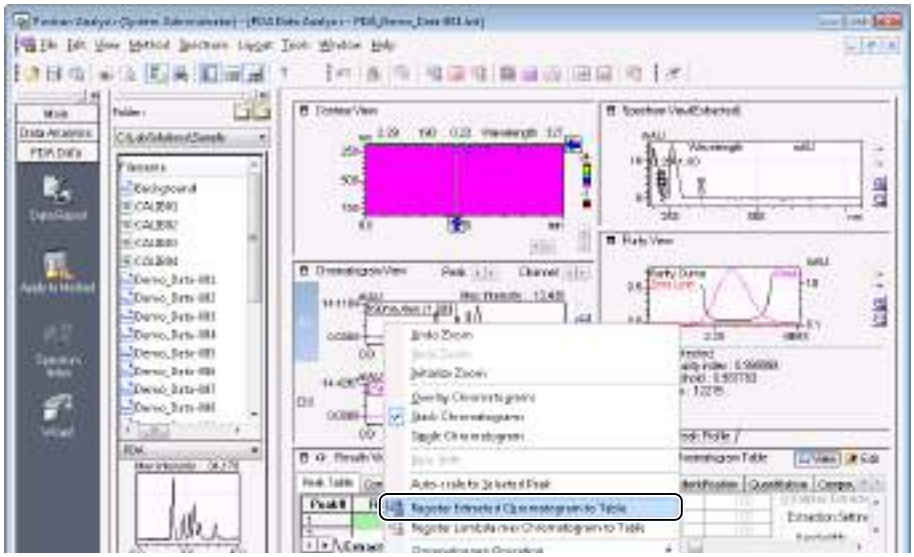
Chromatograms extracted from 3D data can be registered in the Multi-Chromatogram Table.

## 5.2.1 Register Chromatograms to the Multi-Chromatogram Table

Register a chromatogram to the Multi-Chromatogram Table to perform operations such as comparison of multiple chromatograms, output of reports and peak integration.

This section describes how to register chromatograms to the Multi-Chromatogram Table.

**1** **Right-click on the chromatogram in [Ex] (extracted chromatogram), and select [Register Extracted Chromatogram to Table].**



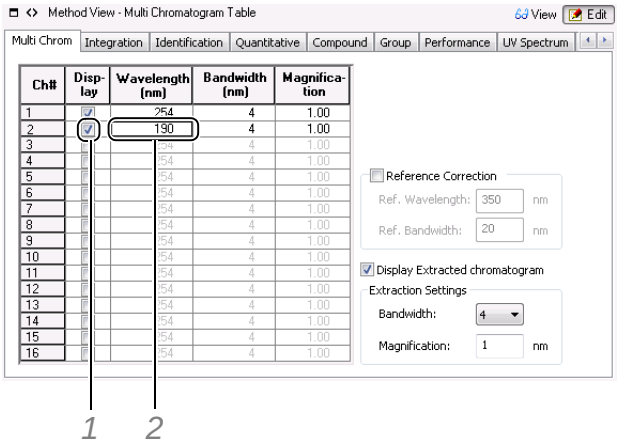
The extracted chromatogram is registered to a channel in the Multi Chromatogram Table.

**NOTE**

- The extracted chromatogram cannot be displayed if [Display Extracted chromatogram] is deselected on the [Multi Chrom] tab in [Method View].
- Right-click on the chromatogram, and select [Register Lambda max Chromatogram to Table] to register the lambda max chromatogram for the target peak to the Multi Chromatogram Table. Then, double-click near the peak top of the target peak in [Chromatogram View]. The chromatogram is registered to the Multi Chromatogram Table.
- If the chromatogram display mode is [Overlay Chromatograms] or [Stack Chromatograms], new chromatogram are displayed in [Chromatogram View] as they are registered to a channel in the Multi Chromatogram Table.

**2** **Click Edit (Edit Mode) in [Method View].**

**3** **Click the [Multi Chrom] tab in [Method View], and select the registered chromatograms.**




1 Select [Display Extracted chromatogram] to display the chromatogram in [Chromatogram View].

2 Click the [Wavelength] cell.

Select [Max Plot] from the [Types of Chromatograms] and enter a [Start Wavelength] and an [End Wavelength] to display that chromatogram as a Max Plot.

**NOTE**

Max Plot refers to the chromatogram obtained by plotting the intensity of the maximum absorbance in the specified wavelength range.

**4** **Click View (View Mode) in [Method View].**

The chromatogram is displayed in [Chromatogram View].

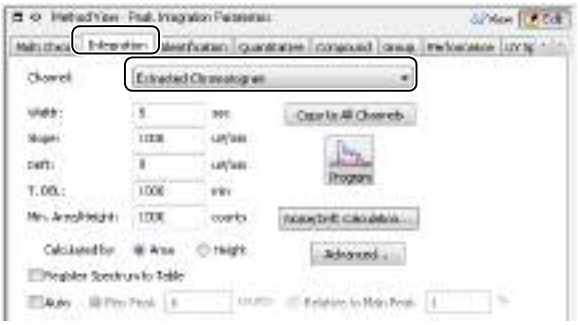
## 5.2.2 Peak Integration Parameters

The peak integration parameters for PDA data can be individually edited for each channel in the Multi Chromatogram Table.

This section describes how to select a channel and perform data processing on that channel.

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Integration] tab, and select the target channel from the [Channel] list.**



**3** **Edit the peak integration parameters.**

**Reference**

Refer to *"4.2 Peak Integration Parameters" P.88* for details on peak integration operations.

**4** **Click View (View Mode) in [Method View].**

The chromatogram in the selected channel is reintegrated with the new peak integration parameters.

**NOTE**

Right-click on the chromatogram in [Chromatogram View], and select [Manual Integration Bar] to manually integrate the chromatograms for each channel. Refer to*"4.2.4 Manual Peak Integration" P.93* for details on manual peak integration.

# 5.3 Register Spectra

Register spectra extracted from 3D data to the Spectrum Table to perform a library search and calculate the similarity between each spectrum and the reference spectrum.

## 5.3.1 Register Spectra to the Spectrum Table

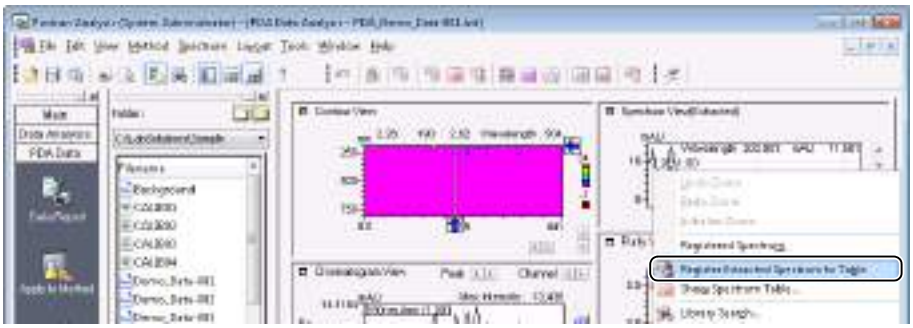
If the displayed spectra are registered to the Spectrum Table, they can be compared with other spectra and their similarity can be calculated.

This section describes how to register extracted spectrum to the Spectrum Table.

**NOTE**

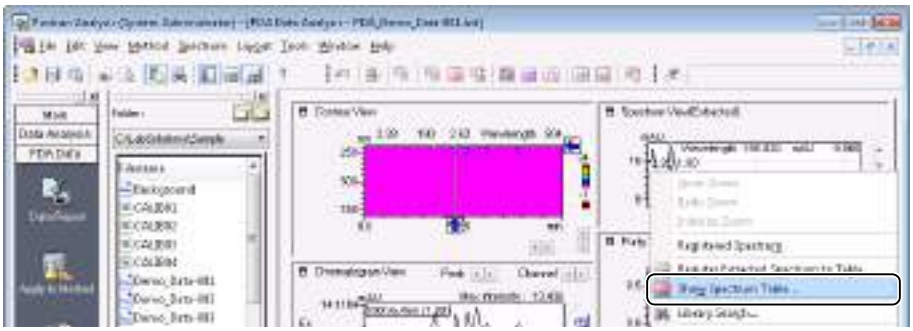
Right-click on the spectrum and select or deselect [Registered Spectrum] and switch between [Spectrum View (Registered)] and [Spectrum View (Extracted)].

**1** **Right-click on [Spectrum View], and click [Register Extracted Spectrum to Table].**



The extracted spectrum is registered to the Spectrum Table.

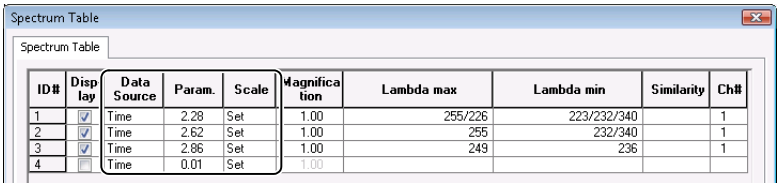
**2** **Right-click on [Spectrum View], and click [Show Spectrum Table].**



**3** **Edit the Spectrum Table.**

*1* Check the content of the [Data Source], [Param.], and [Scale] cells of the registered spectrum.

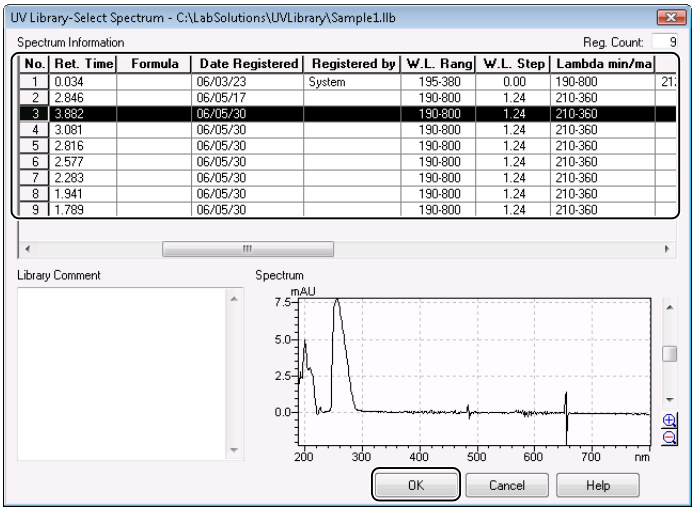
If an extracted spectrum has been registered, [Time] is displayed at [Data Source], and the retention time when it was extracted from the chromatogram is displayed at [Param.].



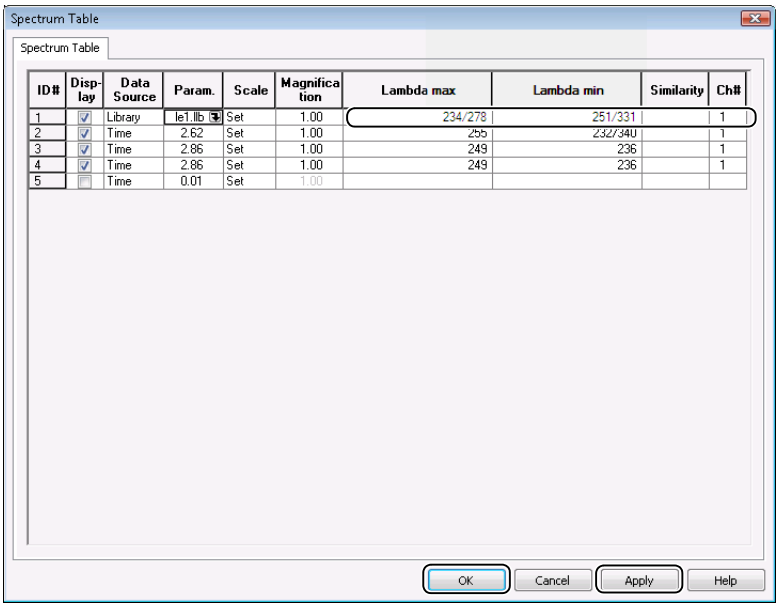

| ID# | Display | Data Source | Param. | Scale | Magnification | Lambda max | Lambda min | Similarity | Ch# |
|---|---|---|---|---|---|---|---|---|---|
| 1 | ☑ | Time | 2.28 | Set | 1.00 | 255/226 | 223/232/340 | | 1 |
| 2 | ☑ | Time | 2.62 | Set | 1.00 | 255 | 232/340 | | 1 |
| 3 | ☑ | Time | 2.86 | Set | 1.00 | 249 | 236 | | 1 |
| 4 | ☐ | Time | 0.01 | Set | 1.00 | | | | |

2 Click the [Data Source] cell and select [Library] and select the UV library file to register a spectrum in a library file to the Spectrum Table.

3 Select the spectrum in the library file from the [UV Library-Select Spectrum] sub-window, and click [OK].



## 4 Click [Apply], check the display in [Spectrum View], and then click [OK].




**NOTE**

- If [Spectrum View (Registered)] is displayed, double-click anywhere in [Chromatogram View] to register the extracted spectrum to the Spectrum Table.
- Select [Register Spectrum to Table] on the [Integration] tab in [Method View] to automatically register the spectrum at all peak top times to the Spectrum Table.

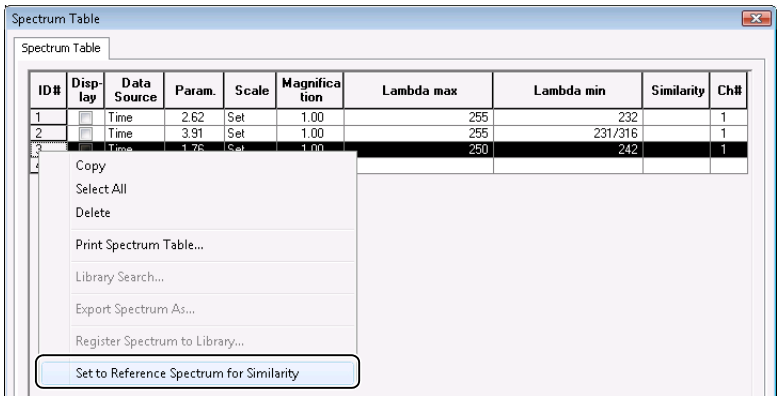
## 5.3.2 Calculate Spectrum Similarity

The similarity between the reference spectrum and another spectrum in the Spectrum Table can be calculated if a reference spectrum ([Ref]) is registered to the Spectrum Table.

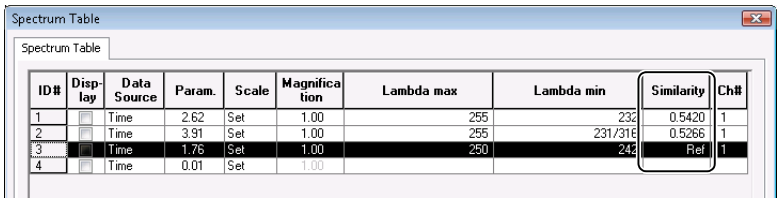
This section describes how to register a reference spectrum to calculate similarity.

**1** **Right-click the ID No. to be used as the reference spectrum, and click [Set to Reference Spectrum for Similarity].**

[Ref] is displayed in the [Similarity] for the selected ID#.




**2** **Click [Apply], and check [Similarity] of the spectrum currently registered to the Spectrum Table.**



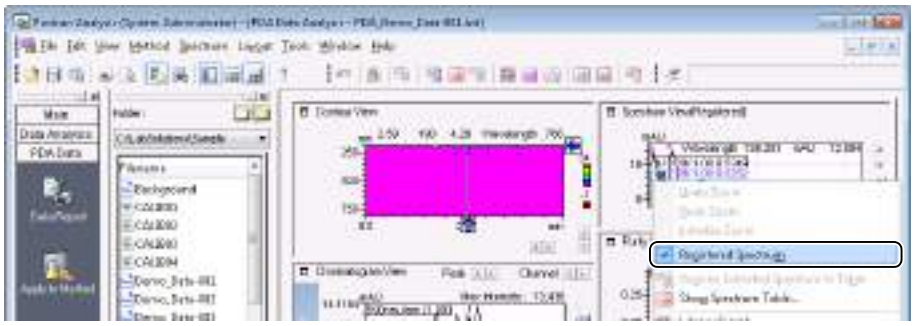

**NOTE**

[Similarity] is displayed as a value with respect to [Ref] = 1.

**3** **Click [OK].**

**NOTE**

Right-click on the [Spectrum View] and select [Registered Spectrum] to display the spectrum currently registered in the Spectrum Table.



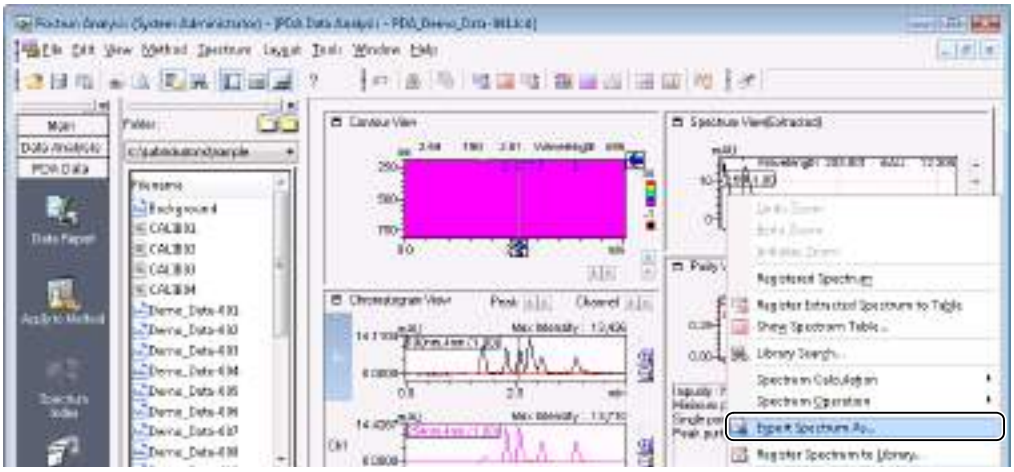
## 5.3.3 Create a Spectrum File

Spectra can be exported to common format (.jcm) files. Exported files are used to register to library files and to perform peak identification based on similarity.

This section describes how to export a spectrum in [Spectrum View] to a file, and how to export spectra registered to the Spectrum Table to files.

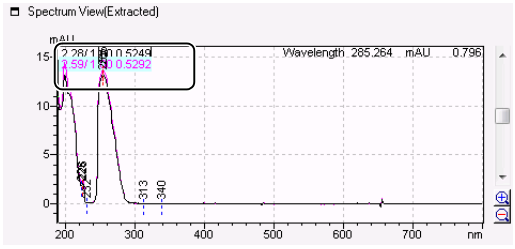
### ■ Export a Spectrum in [Spectrum View]

**1** **Right-click on [Spectrum View], and click [Export Spectrum As].**



**NOTE**

If the view mode is [Spectrum View (Registered)], select the spectrum label before right-clicking on [Spectrum View].

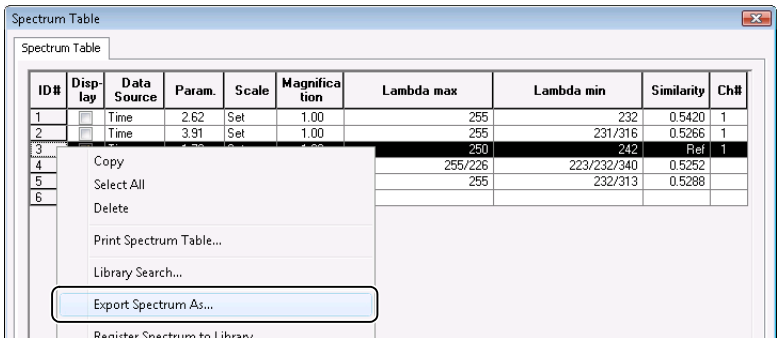



**2** **Enter the file name, and click [Save].**

The spectrum file is created.

## ■ Export Spectra Registered to the Spectrum Table

**1** **Right-click on the ID No. of the spectrum to export, and click [Export Spectrum As].**




**2** **Enter the file name, and click [Save].**

The spectrum file is created.

# 5.4 UV Spectrum Library

A file that contains multiple UV spectra is called a library file. Library file allow for the comparison of unknown spectra to a library of known spectra to identify the unknown compound.

This section describes how to make a library file according to the following procedures.

1. *"Create a Library File"*
2. *"Register a UV Spectrum to the Library File"*
3. *"Edit a Library File"*

**Reference**

Refer to *"5.5.1 Identify Peaks by Spectrum Similarity" P.148* or *"5.5.2 Use [Library Search] to Search for Spectra" P.151* for more details.

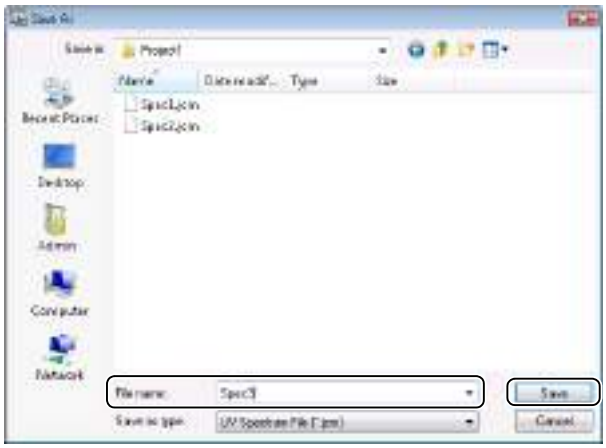
## 5.4.1 Create a Library File

A UV spectra library file must be created before extracted spectra can be added to it.

**1** **Click the (UV Library Editor) icon on the [Main] assistant bar in the [Postrun Analysis] program.**

**2** **Click (New) on the toolbar.**

**3** **Enter a [File name], and click [Save].**



The UV library file is created.

## 5.4.2 Register a UV Spectrum to the Library File

This section describes how to register the UV spectra displayed in the [Spectrum View] and spectra files to the library file made in *"5.4.1 Create a Library File"*.



### ■ Register a UV Spectrum File

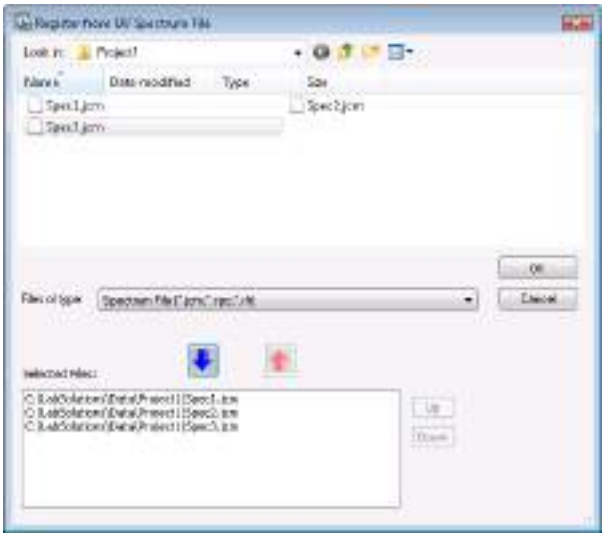
**Reference**

Refer to *"5.3.3 Create a Spectrum File" P.140* for details.

**1** **Right-click on [Spectrum Information] in the [UV Library Editor] window, and click [Register from UV spectrum file].**

**2** **Select the desired UV spectrum file and then click .**

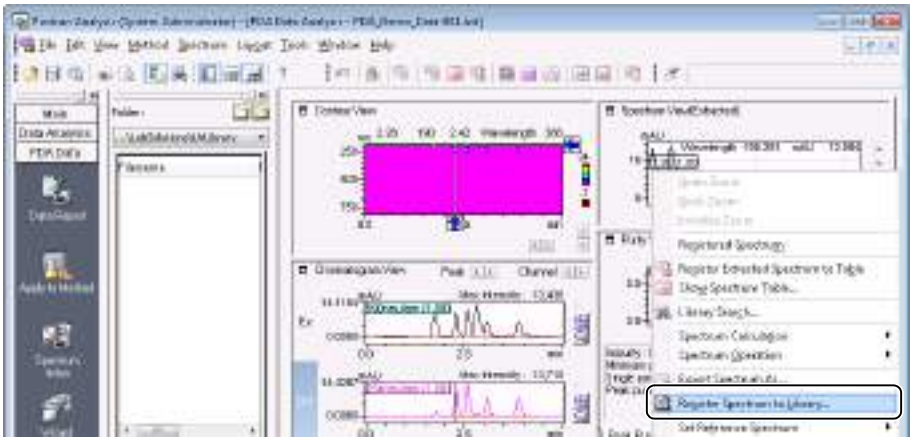
The UV spectrum file name is displayed in the [Selected Files] box. Repeat this procedure to select all files required for the UV library.



The selected UV spectra files are registered to the UV library file.

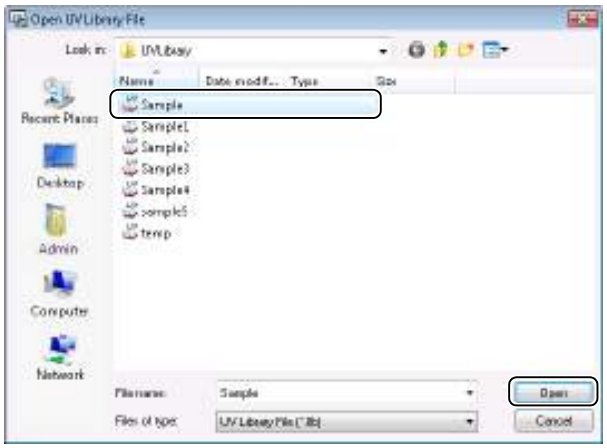
## ■ Register a UV Spectrum

**1** **Right-click on [Spectrum View] in the [PDA Data Analysis] window, and click [Register Spectrum to Library].**



The spectrum is added to the UV library file.

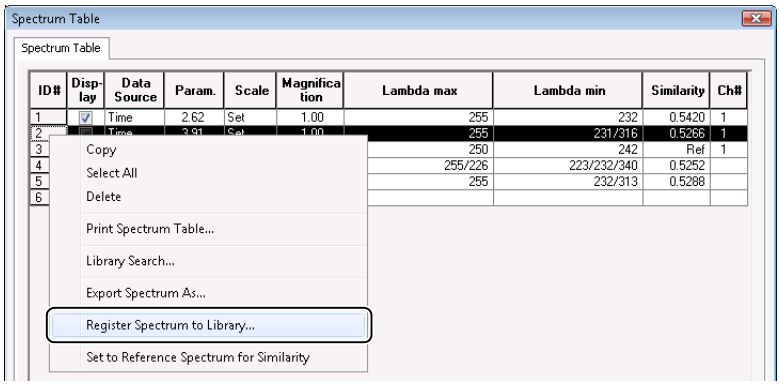
## 2 Select the desired UV library file, and click [Open].



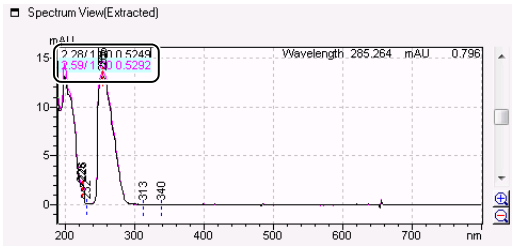

The spectrum is added to the UV library file.

### NOTE

- Right-click on the ID No. of the desired spectra, and select [Register Spectrum to Library] to add spectra in the Spectrum Table to the library file.




- If the view mode is [Spectrum View (Registered)], select the spectrum label before right-clicking on [Spectrum View], and then select [Register Spectrum to Library].



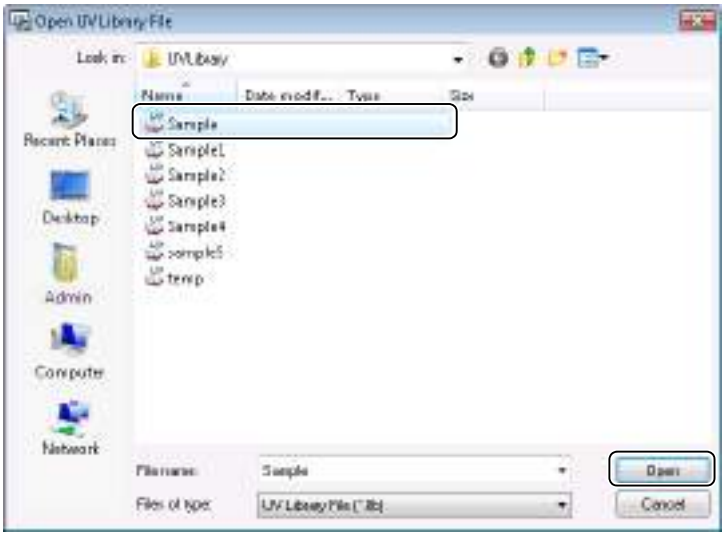
## 5.4.3 Edit a Library File

This section describes how to edit the spectrum files registered at *"5.4.2 Register a UV Spectrum to the Library File"*.

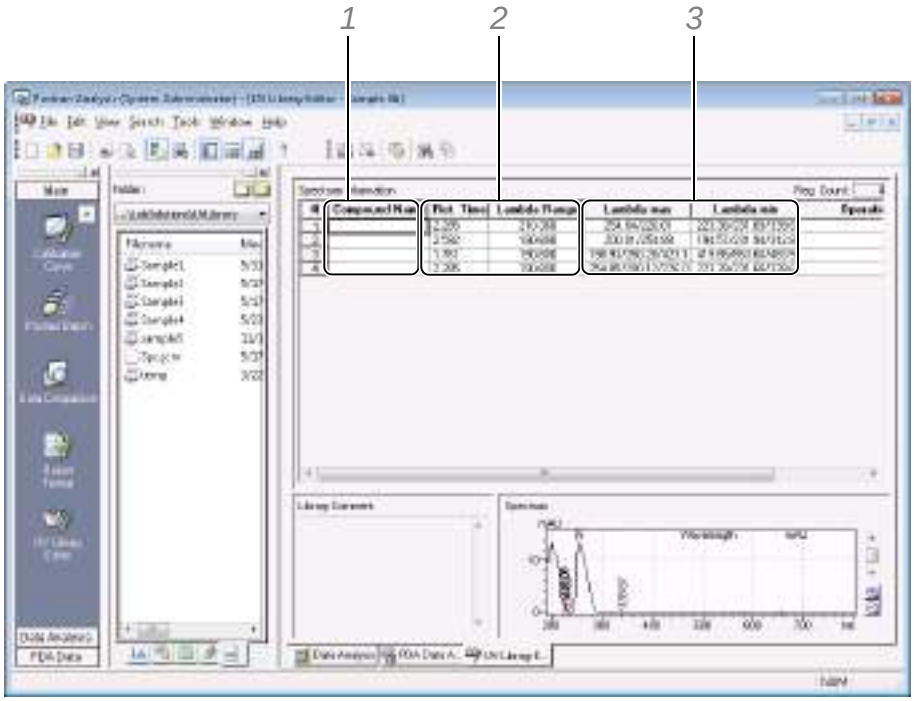
**1** **Click the (UV Library Editor) icon on the [Main] assistant bar in the [Postrun Analysis] program.**

**2** **Click the (Open) button on the toolbar.**

**3** **Select the desired UV library file, and click [Open].**



## 4 Edit the [Spectrum Information] in the UV library file.




1 Enter the [Compound Name] if one was not already entered.
2 Enter the wavelength range in the [Lambda Range] column for use the library search.
3 Check the [Lambda max] and [Lambda min] values.

**NOTE**
The items displayed at [Spectrum Information] can be edited with [Table Style].
Right-click on [Spectrum Information], and select [Table Style].

## 5 Click the (Save) button on the toolbar.

The UV library file is saved.

# 5.5 Specify a Compound From a Spectrum

Compare the spectra of known compounds with the spectrum of an unknown compound to identify and specify the compounds from a spectrum.

This section describes the following operations.

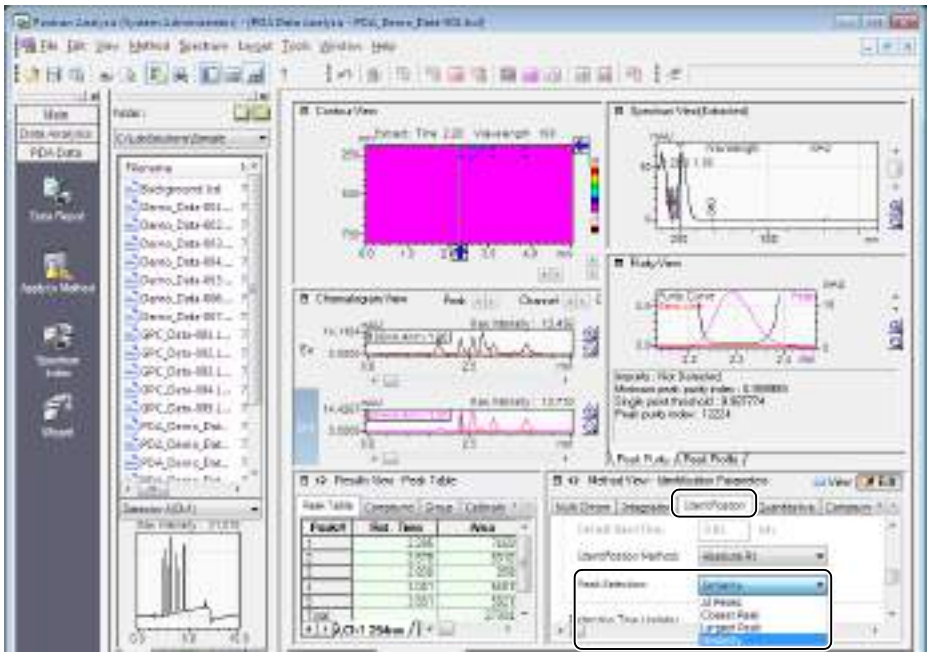
- *"Identify Peaks by Spectrum Similarity"*
- *"Use [Library Search] to Search for Spectra"*
- *"Spectrum Conditions of the Search Target"*

Set the spectrum conditions of the search target to perform higher precision similarity and library searches.

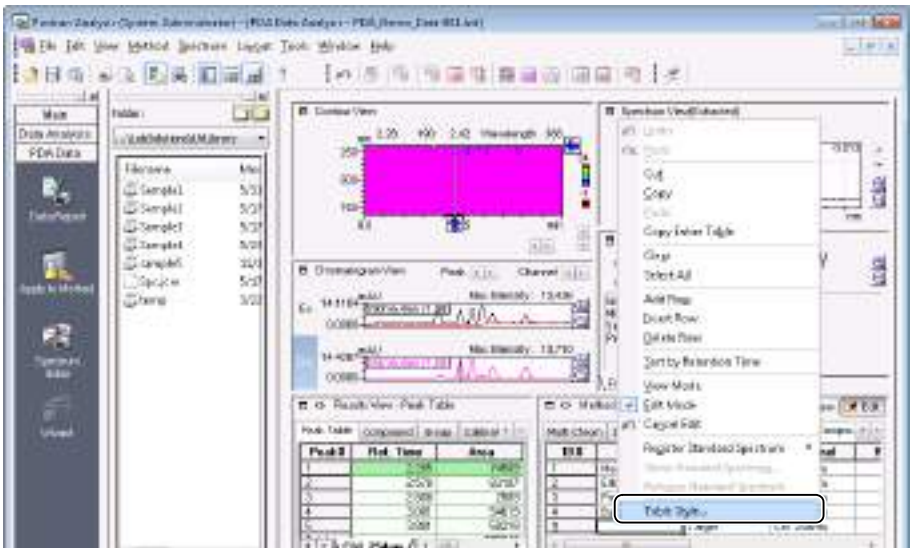
## 5.5.1 Identify Peaks by Spectrum Similarity

**1** **Click Edit (Edit Mode) in [Method View].**

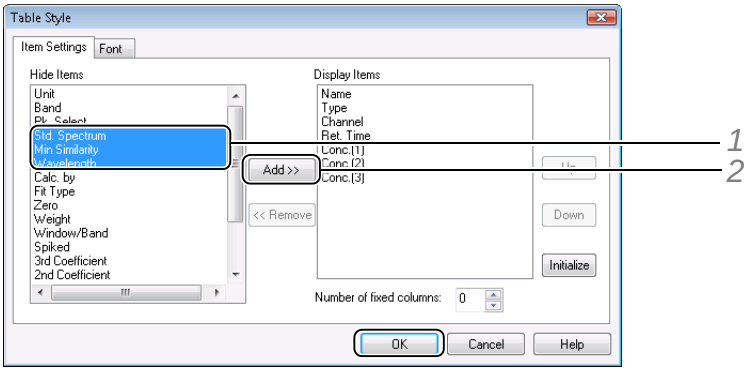
**2** **Click the [Identification] tab, and select [Similarity] in the [Peak Selection] list.**



## 3 Click the [Compound] tab, right-click on the Compound Table, and click [Table Style].



## 4 Make the settings in the [Table Style] sub-window, and click [OK].




*1* Select [Std. Spectrum], [Min Similarity], and [Wavelength] in the [Hide Items] box.

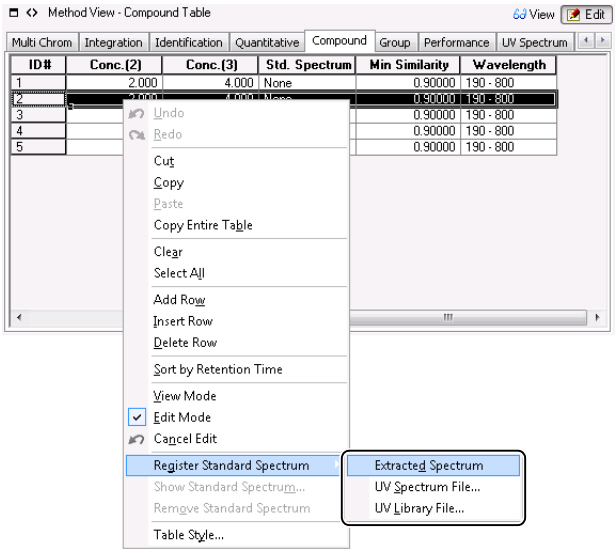
*2* Click [Add].

[Std. Spectrum], [Min Similarity], and [Wavelength] are added to the [Display Items] box.

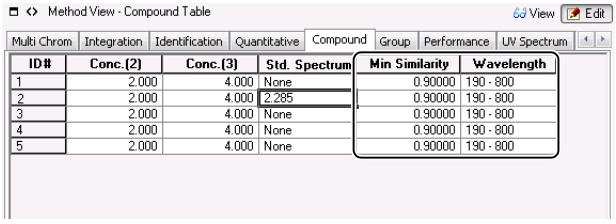
**NOTE**

Change the display order of items in the Compound Table, by selecting the item in the [Display Items] box and then clicking [Up] or [Down].

**5** **Right-click the [ID#] of the compound whose similarity is to be identified, click [Extracted Spectrum], [UV Spectrum File] or [UV Library File] at [Register Standard Spectrum], and register the standard spectrum for the compound.**




**6** **Enter the [Min Similarity] and [Wavelength] that is associated with the [Std. Spectrum].**




**7** **Click View (View Mode) in [Method View].**

**NOTE**

- Right-click and select [Show Standard Spectrum] to check a registered spectrum.
- The peak is not identified if the similarity between the standard spectrum and the spectrum of the time at the top of the detected peak falls below the threshold.

## 5.5.2 Use [Library Search] to Search for Spectra

This section describes how to perform a library search.

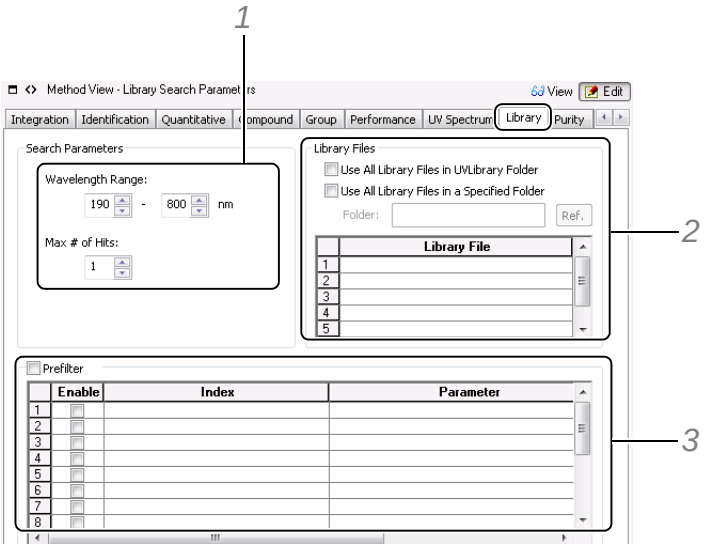
1. Set library search criteria
2. Execute the library search

### ■ Library Search Criteria

The following example describes how to set the criteria to search the similarity between an unknown spectrum and the spectra registered to the library file.

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Library] tab, and enter the search criteria.**




*1* Set the [Wavelength Range] and [Max # of Hits].

**NOTE**

[Max # of Hits] is the number of spectra to display in the [UV Library Search Results] sub-window.

*2* Set the [Library Files] parameters.

**NOTE**

- Select [Use All Library Files in UVLibrary Folder] to search all of the library files in the UVLibrary folder.
- Select [Use All Library Files in a Specified Folder] and specify a folder to search all of the library files in a specific folder in the UVLibrary.

*3* Select [Prefilter] and [Enable], then click the [Index] cell and select a keyword to further filter the search results by compound name, retention time or another keyword.

**3** **Click View (View Mode) in [Method View].**

## ■ Execute the Library Search

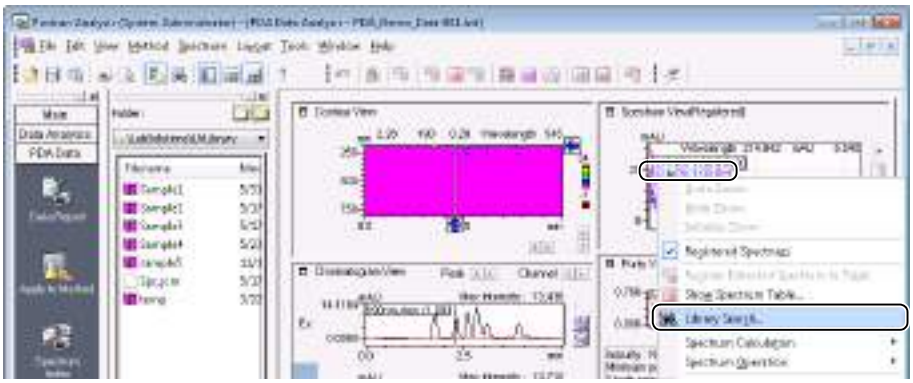
When the library search is executed, matching spectra are displayed in order from the highest similarity to the lowest in the [UV Library Search Results] sub-window.

The following example describes how to select a spectrum in [Spectrum View (Registered)] and perform a library search.

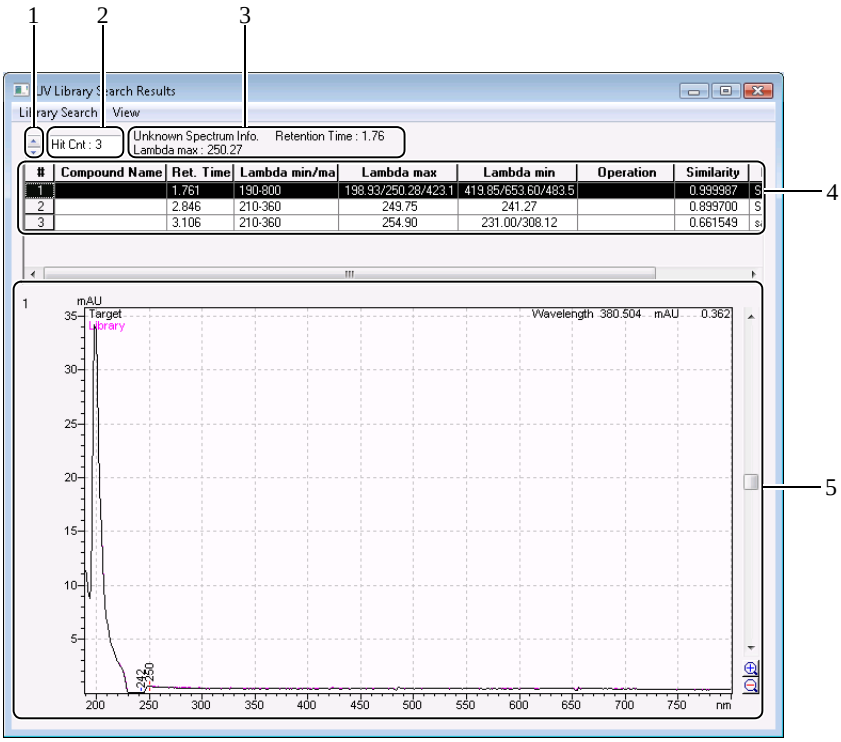
**NOTE**

To perform a library search on the extracted spectrum, first, display the spectrum extracted from [Contour View] or [Chromatogram View] in [Spectrum View (Registered)], and execute the library search.

**1** **Select the spectrum in the [Spectrum View], right-click on the view, and click [Library Search].**



The spectra found (hit) by the search criteria are displayed in the library search results. The following sub-window displays search results when the [Max # of Hits] is set to “3”.



| No. | Explanation |
|---|---|
| 1 | Changes the spectrum displayed in the graph.<br>The number of graphs to display can be set at [Display Settings] on the [View] menu. |
| 2 | Determines the number of hits displayed in the search results window. |
| 3 | Displays the [Ret. Time] and [Lambda max] values for the UV spectrum of the target peak. |
| 4 | Displays a table of spectrum information that was hit (found) in the search.<br>The spectrum information is displayed in order from the highest similarity to lowest. |
| 5 | Displays the searched spectra (Library) overlaying the unknown spectra (Target). |

**NOTE**

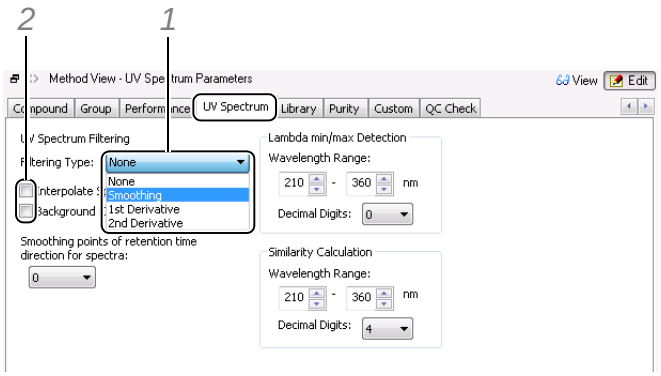
Click [Repeat Search] on the [Library Search] menu, and change the search criteria in the [Library Search] sub-window to perform the search again with new criteria.

## 5.5.3 Spectrum Conditions of the Search Target

Set the spectrum conditions during extraction of the UV spectrum to perform higher precision peak identification and library searches.

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [UV Spectrum] tab, and set the spectrum conditions.**




*1* Select [Smoothing] in the [Filtering Type] list to perform spectral smoothing.

*2* Select [Background Compensation] to perform background compensation on spectra.

**3** **Click View (View Mode) in [Method View].**

# 5.6 Peak Purity Analysis

The peak purity can be calculated and the peak shape of chromatograms at each wavelength can be compared to check whether detected peaks contain impurities.

**Reference**

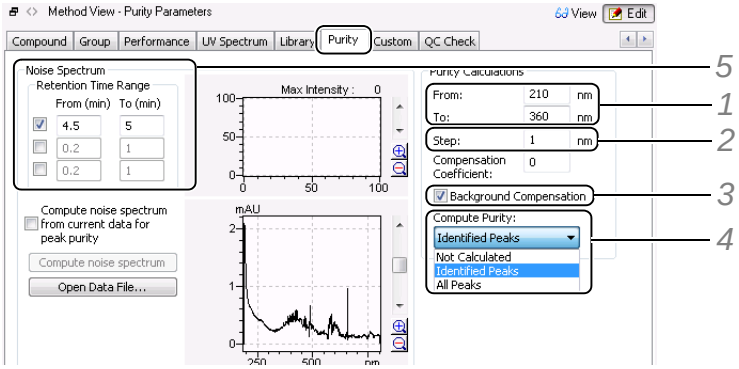
Refer to Help for details on peak purity analysis.

## 5.6.1 Peak Purity Calculation Parameters

This section describes how to set the calculation range and the compensation conditions based on the noise spectrum.

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Purity] tab, and set the conditions for the peak purity calculation.**




*1* At [From] and [To], enter the wavelength range where purity will be calculated.

*2* At [Step], enter the wavelength interval to use for the calculation.

*3* Select [Background Compensation].

**NOTE**

- Select [Background Compensation] to calculate the peak purity of components with a slow retention time or whose baseline easily drifts as in gradient acquisition.
- Insufficient peak separation causes the start and end points of the peak to overlap. Better results are obtained by not performing background compensation.

*4* Select [Identified Peaks] from the [Compute Purity] drop-down list.

**NOTE**

Depending on the number of peaks and whether [All Peaks] is selected, it may take time to perform data analysis.

*5* At [From] and [To], enter the retention time range to set as the noise spectrum.

Select a time range that incorporates the retention time of the target component.

**NOTE**

- Display the chromatogram as a Max Plot, and verify that there are no peaks between [From] and [To], then select the noise spectrum range.
- Select [Compute noise spectrum from current data for peak purity] to compute the noise spectrum from the every data file.

**3** **Click View (View Mode) in [Method View].**

The purity calculation is executed according to the preset conditions.

## 5.6.2 Displaying Calculation Results

[Purity View] has 2 sub-windows for viewing the results of the peak purity calculation, [Peak Purity] and [Peak Profile].

[Peak Purity] is used to check the peak purity based on the spectrum information of the detected peak. [Peak Profile] is used to check for impurities by comparing chromatograms at multiple wavelengths.

First, select the desired peak in [Chromatogram View] or [Contour View]. This section describes how to select peaks whose purity is to be checked in [Chromatogram View].

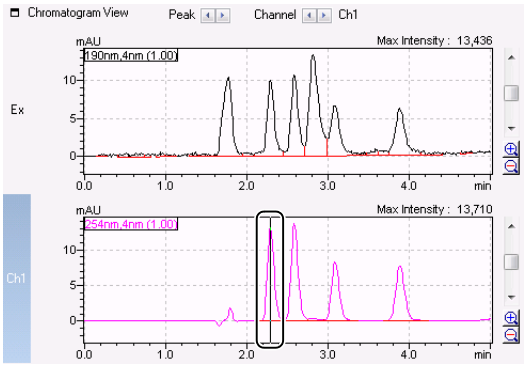
Next, check the calculation results at [Purity View]. The section describes the following 2 methods:

- *"Display Calculation Results using the 3-Point Peak Purity Method"*
- *"Display the Calculation Result using the Total Peak Purity Method"*

**1** **Move the extraction line in [Chromatogram View], to the peak for which purity is to be calculated.**

**Reference**

Refer to *"Display the Spectrum of a Desired Retention Time Extracted from the Chromatogram" P.132* for more details.

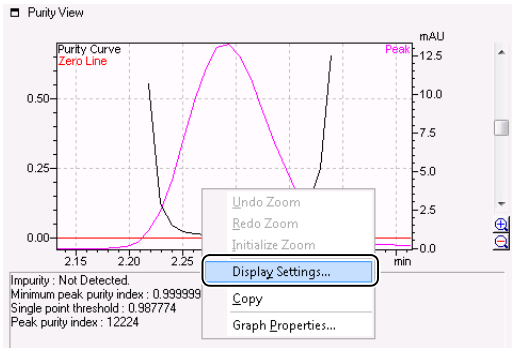



If the peak is detected, the purity of the selected peak is calculated.

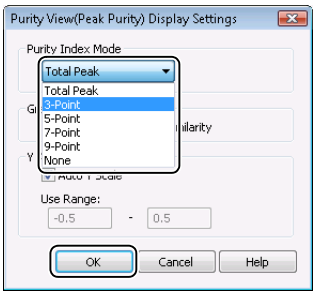
### ■ Display Calculation Results using the 3-Point Peak Purity Method

Peak purity is calculated based on 3 points, the upslope, peak top point and downslope.

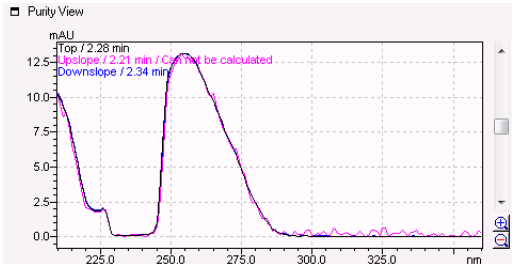
**1** **Select the [Peak Purity] tab in [Purity View] then right-click the graph and select [Display Settings].**



**2** **Select [3-Point] from the [Purity Index Mode] drop-down list, and click [OK].**




**3** **Confirm that the 3-point spectra method waveform and calculation results are displayed.**



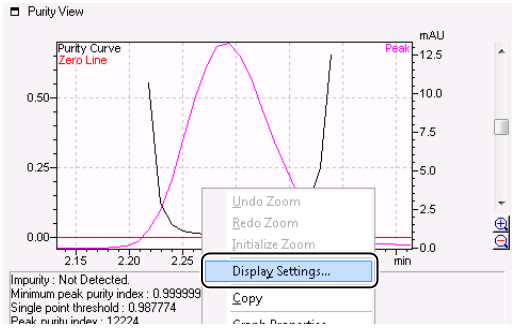

**NOTE**

If the spectral similarity between the peak top, the upslope and the downslope is higher than the threshold, it is an indication that the calculated peak does not contain impurities.

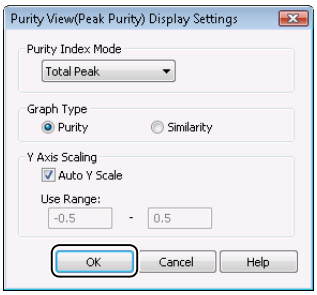
## ■ Display the Calculation Result using the Total Peak Purity Method

Peak purity is calculated based on all of the points from peak start to peak end, then the similarity and purity curves are displayed.

**1** **Select the [Peak Purity] tab in [Purity View] then right-click the graph and select [Display Settings].**



## 2 Select [Total Peak] from the [Purity Index Mode] drop-down list, and set the [Graph Type] and [Y Axis Scaling], and click [OK].

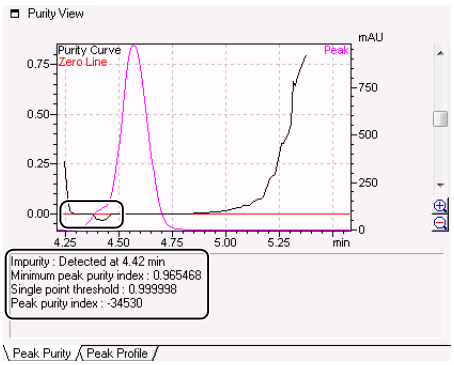



**NOTE**

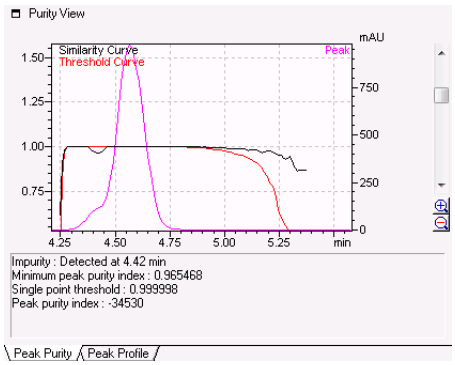
- If [Purity] is selected, the purity curve (curve obtained by subtracting the threshold curve from the similarity curve) and zero compensation line are displayed in the graph.
- If [Similarity] is selected, the similarity curve and threshold curve are displayed in the graph.
- To change the display scale of the similarity curve, deselect [Auto Y Scale] at [Y Axis Scaling], and enter a display range.
  In the following example, the display range is set to 0.99 to 1.01.
- Notice in the following [Purity] graph example that impurities are detected where the purity curve is below the zero compensation line.
  The negative [Peak purity index] value confirms that the sample contains impurities.

The [Purity] graph or [Similarity] graph is displayed.

Purity graph



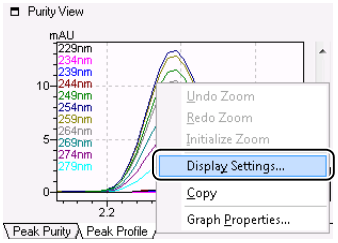

Similarity graph



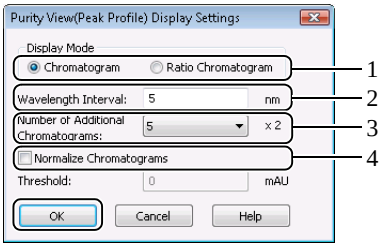
## ■ Examine Chromatograms using the Peak Profile

Display chromatograms at multiple wavelengths to compare peak shape.

**1** **Select the [Peak Purity] tab in [Purity View] then right-click the graph and select [Display Settings].**




**2** **Enter the parameters in the [Display Settings] sub-window, and click [OK].**

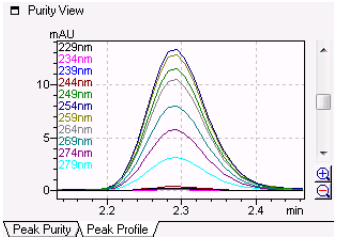



*1* Select the [Display Mode].

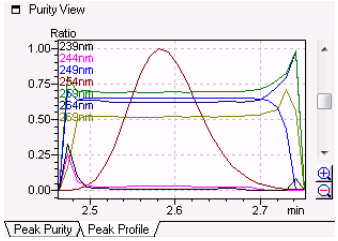
| No. | Explanation |
|---|---|
| 1 | Select [Chromatogram] to display the chromatogram based on the [Wavelength Interval] and [Number of Additional Chromatograms] parameters.<br>Select [Ratio Chromatogram] to display the central wavelength chromatogram with the ratios between the chromatograms based on the [Wavelength Interval] and [Number of Additional Chromatograms]. |
| 2 | Select how many wavelengths (nm) will separate the chromatograms displayed on the short and long sides of the center wavelength. |
| 3 | Select the number of chromatograms to display on the short and long sides of the center wavelength. Up to 5 wavelengths can be specified on each side. |
| 4 | If [Chromatogram] is selected as [Display Mode] and [Normalize Chromatograms] is selected, the intensity axis of the chromatogram is normalized. |

The [Chromatogram] or [Ratio Chromatogram] is displayed.

Chromatogram




Ratio chromatogram




**NOTE**

The center wavelength refers to the wavelength of the chromatogram extracted from the contour view or set in the Multi Chromatogram Table.

# 5.7 Print PDA Data Analysis Results

A report format file must be made in the [Report] window to print PDA data analysis results. This software provides several report format files to make printing easier. First-time users of this software can easily print analysis results using the pre-installed report format files. As users becomes more familiar with the software operations, they can edit or add report items to the pre-installed report format files, or create a new report format file and use it to print reports.

This chapter describes the following procedures.

- *"Open the [Report] Window"*
- *"Open Report Format Files"*
- *"Edit PDA Report Format"*
- *"Preview Before Printing"*
- *"Save Report Format Files"*

## 5.7.1 Open the [Report] Window

Open the [Report] window in either the [Realtime Analysis] program or the [Postrun Analysis] program.

This section describes how to open the [Report] window in the [Postrun Analysis] program.



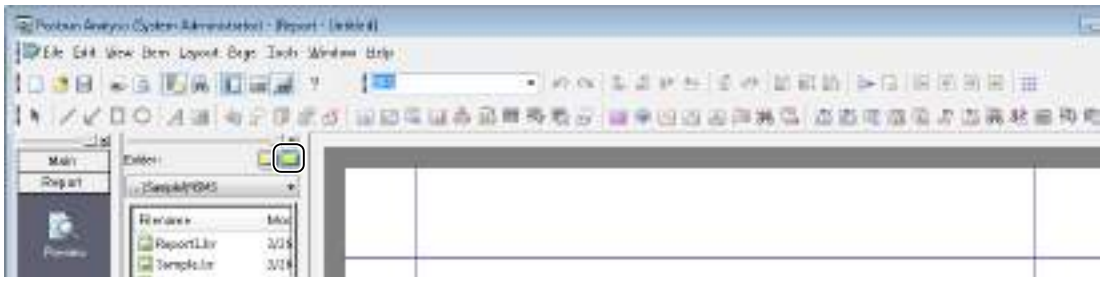
**1** **Click the (Report Format) icon on the [Main] assistant bar in the [Postrun Analysis] program.**

The [Report] window opens.

## 5.7.2 Open Report Format Files

Several report format files are pre-installed in the \LabSolutions\Sample\LC folder. This section describes how to open the report format file “PDADataAnalysisResults.lsr”.

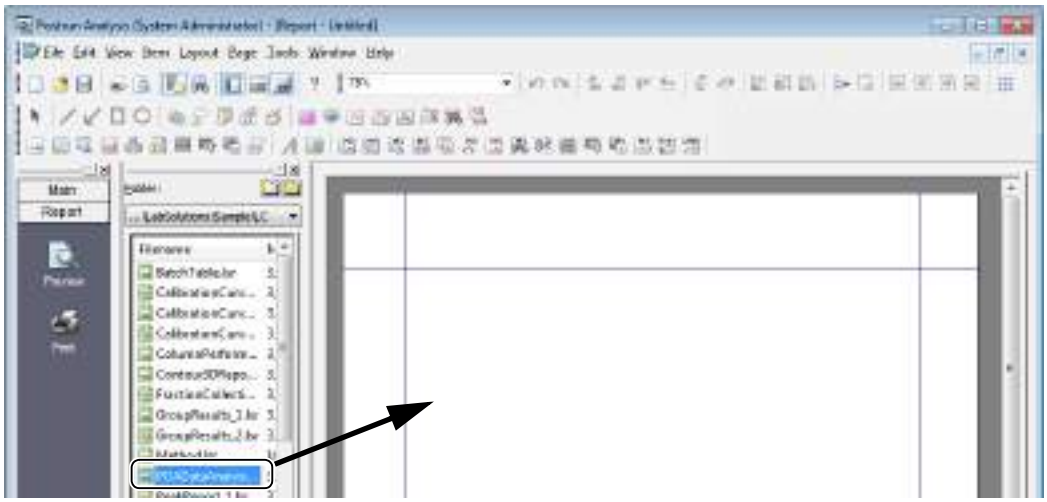
**1** **Click (Select Folder) in the [Data Explorer] sub-window.**



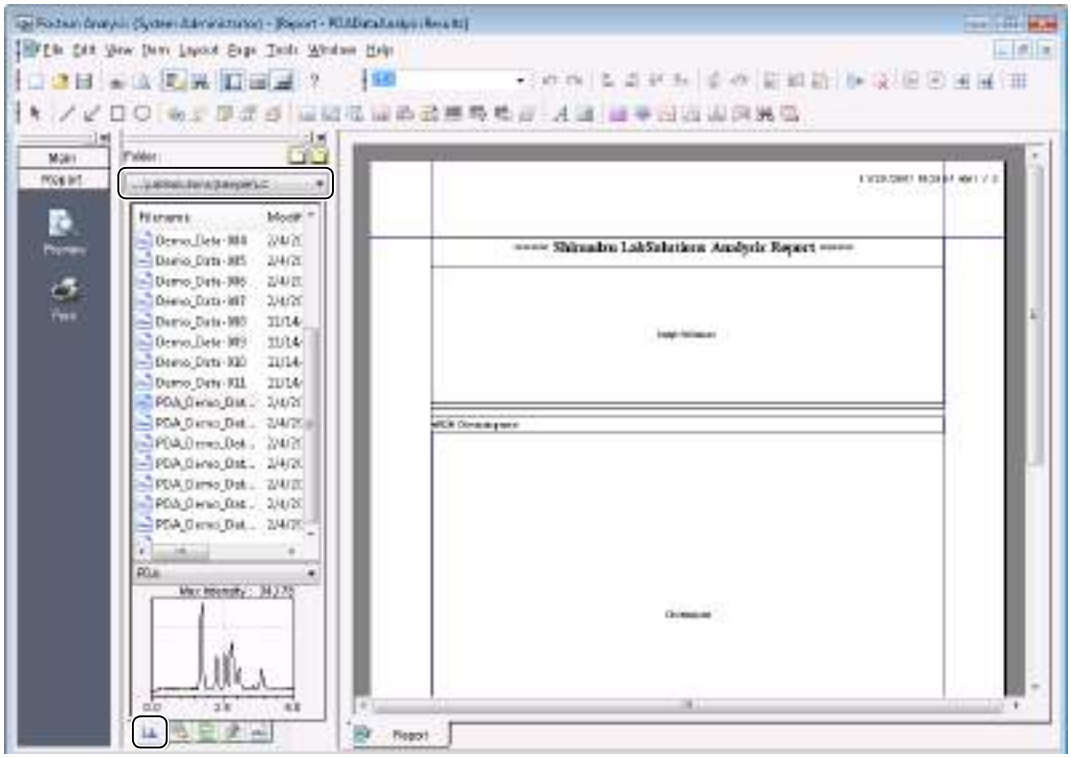
**2** **Select “\LabSolutions\Sample\LC”, and click [Close].**

The “\LabSolutions\Sample\LC” folder is displayed in the [Data Explorer] sub-window.

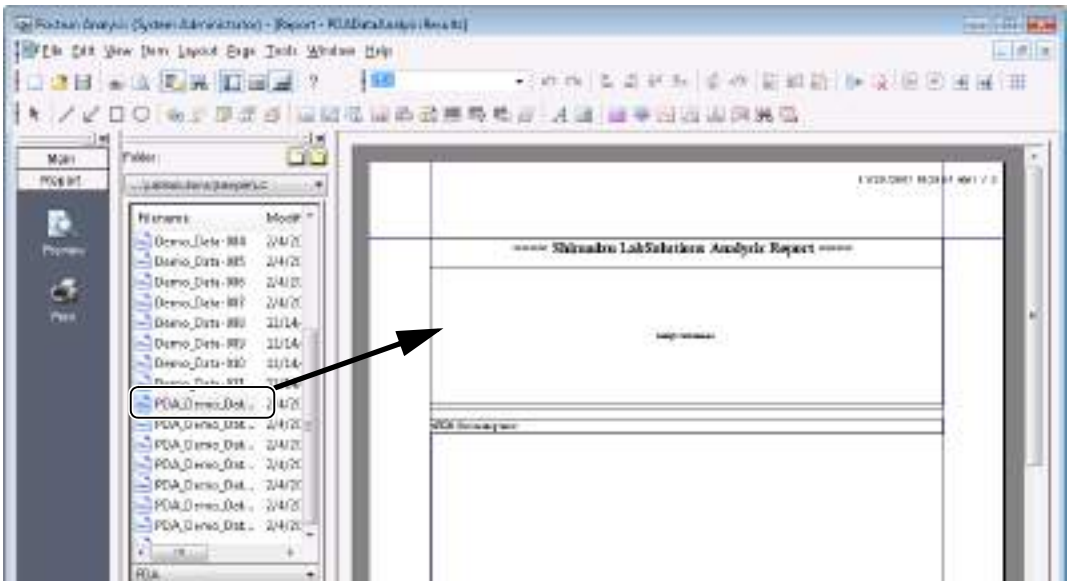
**3** **Drag-and-drop “PDADataAnalysisResults.lsr” onto the [Report] window.**



**4** **Click the (Data) tab in the [Data Explorer] sub-window, and select the appropriate data file folder.**

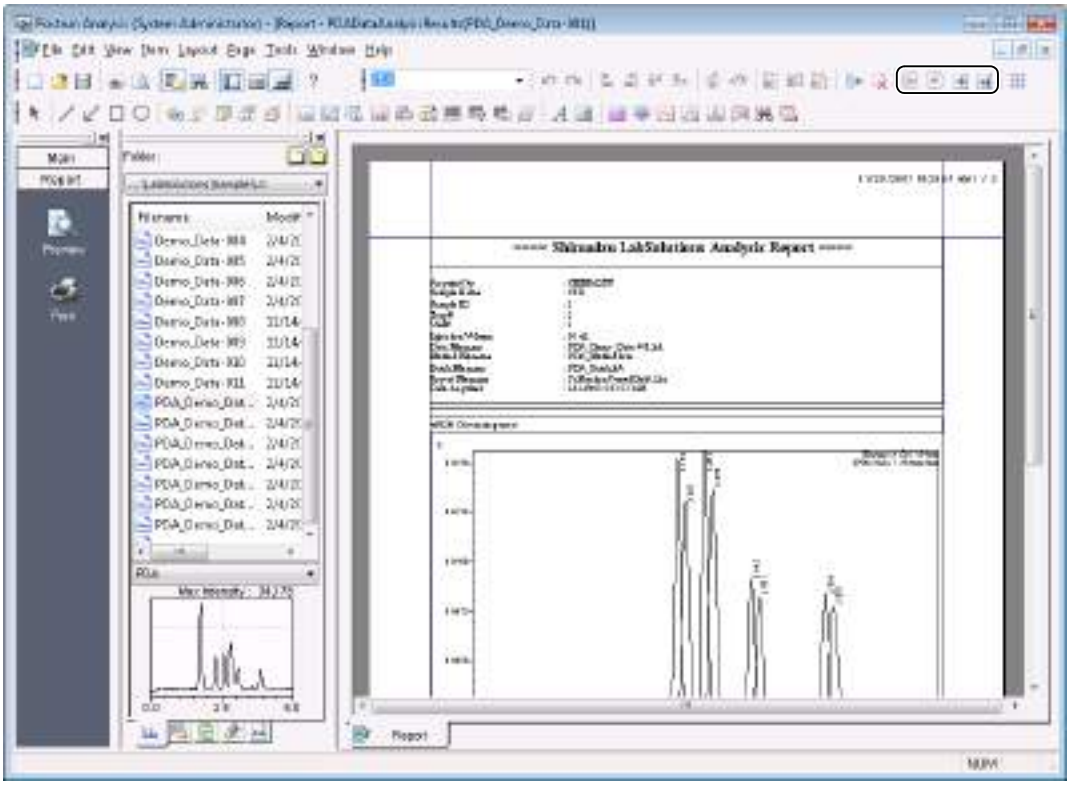


## 5 Drag-and-drop the data file into the report format.



The data file is loaded into the report format and displayed.

## 6 If the report includes multiple pages, use the icons on the toolbar to review the content of the other pages.

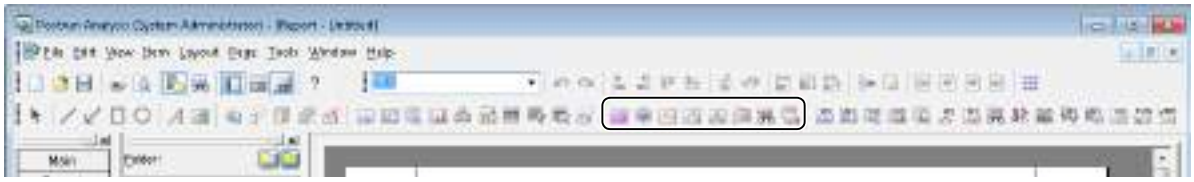


**NOTE**

If the desired data file is not displayed in the [Data Explorer] sub-window, click (Select Folder), and specify the folder that contains the desired data file.

## 5.7.3 Edit PDA Report Format

The following 8 report items are provided for inclusions in the PDA data analysis format.



| Item | Contents |
|---|---|
| Contour Graph | Prints the contour graph and 3D graph of the data acquired by the PDA detector.<br>**Reference**<br>For details, see *"Change the Display Color and Scale of the Contour View" P.164*. |
| 3D Graph | |
| UV Spectrum | Prints the information in the spectrum files and the spectra extracted from the data acquired by the PDA detector.<br>**Reference**<br>For details, see *"Change the Content and Print Scale for UV Spectra" P.166*. |
| Peak Purity | Prints the peak purity calculation results for the data acquired by the PDA detector.<br>**Reference**<br>For details, see *"Specify the Peaks and Calculation Method to Print the Peak Purity Calculation Results" P.170*. |
| Peak Profile | |
| UV Spectrum Index | Prints the identified peak information and its spectrum. |
| UV Library Search | Prints the library search results for the data acquired by the PDA detector.<br>**Reference**<br>For details, see *"Change the Content and Print Scale for Library Search Results" P.168*. |
| UV Library | Prints a list of the spectrum information registered to the UV spectrum library. |

This section describes how to edit items in the report format file opened at *"5.7.2 Open Report Format Files"*.

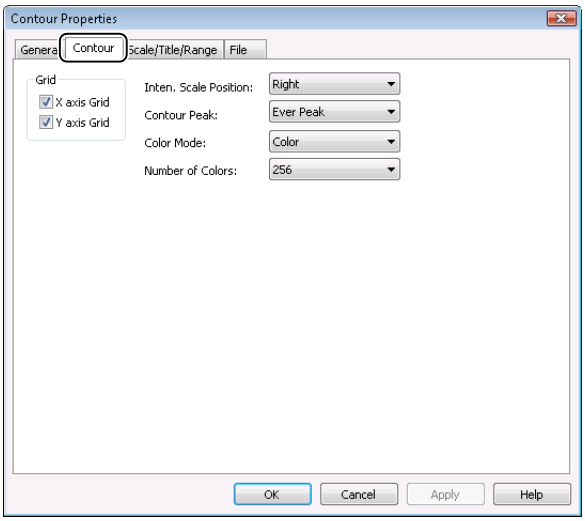
## ■ Change the Display Color and Scale of the Contour View

Use the pre-installed report format file “Contour3DReport.lsr” to print contour views. Refer to *"5.7.2 Open Report Format Files"* and open “Contour3DReport.lsr”.

**1** **Double-click the [Contour Graph] item.**

The [Contour Properties] sub-window is displayed.

**2** **Click the [Contour] tab, and set the [Inten. Scale Position], [Color Mode], and [Number of Colors] parameters.**




**3** **Click the [Scale/Title/Range] tab, then under the [Display Area] deselect [Auto] for the the X-axis (time), Y-axis (wavelength) and Z-axis (intensity). Enter the desired scale for each.**

**4** **Click [OK].**

**Reference**

For details, see *"5.7.4 Preview Before Printing" P.172*.

## ■ Change the Display Scale of 3D Graphs

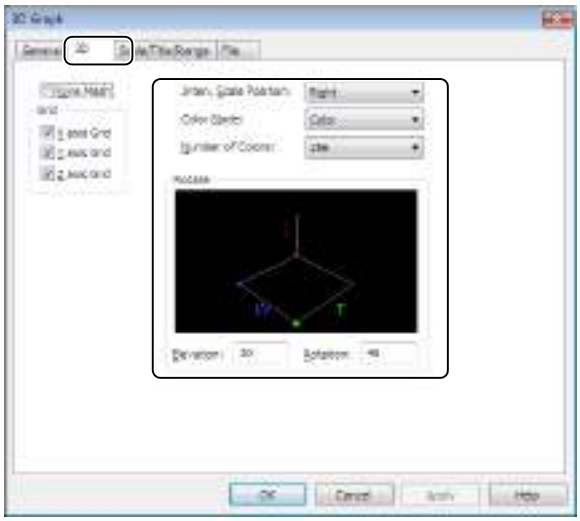
Use the pre-installed report format file “Contour3DReport.lsr” to print 3D graphs. Refer to *"5.7.2 Open Report Format Files"* to open “Contour3DReport.lsr”.

**1** **Double-click the [3D Graph] item.**

**NOTE**

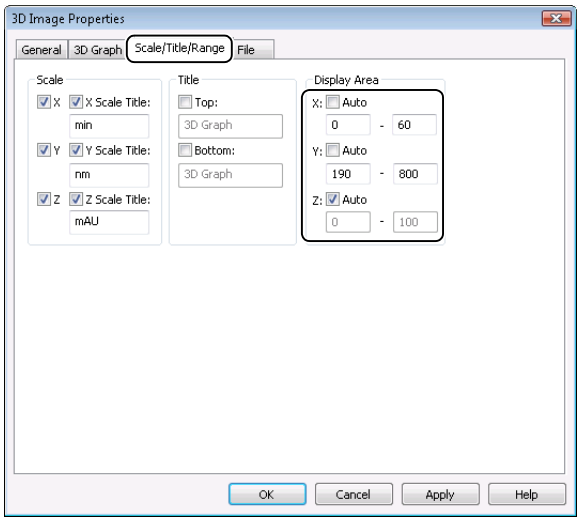
The [3D Graph] item is located on the second page of “Contour3DReport.lsr”.

**2** **Click the [3D] tab, and set the [Inten. Scale Position], [Color Mode], [Number of Colors], and [Rotate] parameters.**



The point of rotation is not displayed.

**3** **Click the [Scale/Title/Range] tab and under the [Display Area], deselect [Auto] for the X-axis (time), Y-axis (wavelength) and Z-axis (intensity). Enter the desired scale for each.**




**4** **Click [OK].**

**Reference**

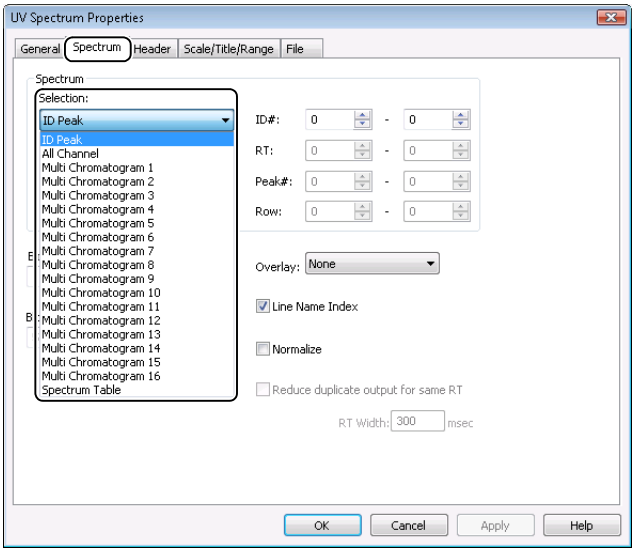
For details, see *"5.7.4 Preview Before Printing" P.172*.

## ■ Change the Content and Print Scale for UV Spectra

Use the pre-installed report format file “PDADataAnalysisResults.lsr” to print UV spectra. Refer to *"5.7.2 Open Report Format Files"* to open “PDADataAnalysisResults.lsr”.

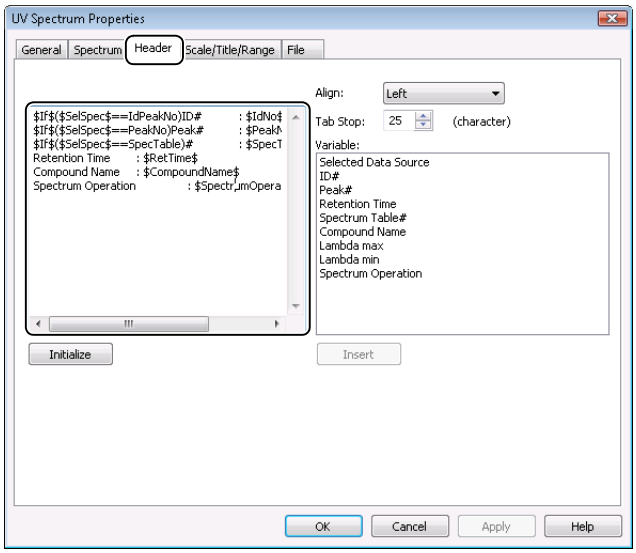
**1** **Double-click the [UV Spectrum] item.**

**2** **Click the [Spectrum] tab, and select the spectrum from the [Selection] list.**

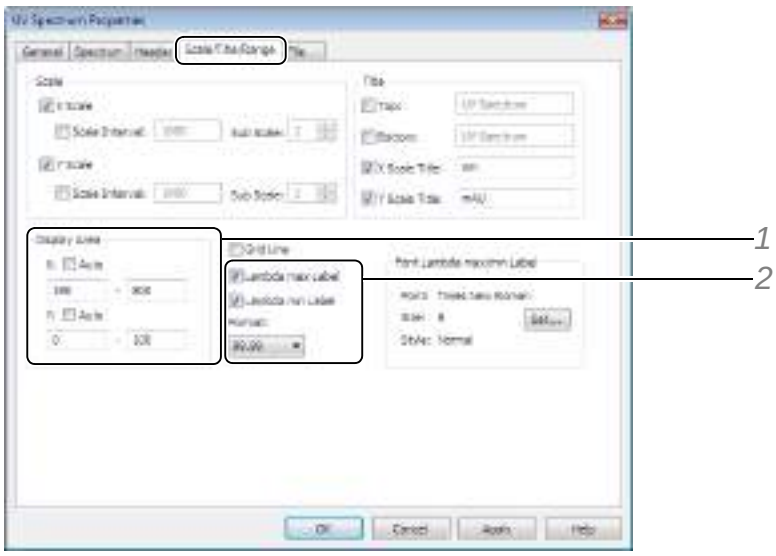



| Parameter | Explanation |
|---|---|
| ID Peak | Selects the spectra to print by entering the ID#s of the compounds in the Compound Table.<br>The spectra of all identified peaks are printed if [0]-[0] is entered. |
| All Channel | Select the retention time range at [RT].<br>The spectra of all detected peaks are printed if [0]-[0] is entered.<br>If multiple peaks are detected, the printed spectra can be easily checked by selecting [Reduce duplicate output for same RT]. |
| Multi Chromatogram | Sets the number of the peak at [Peak #].<br>The spectra of all detected peaks are printed if [0]-[0] is entered. |
| Spectrum Table | Sets the row No. of the table at [Row].<br>All of the spectra registered in the Spectrum Table are printed if [0]-[0] is entered. |

**3** **Click the [Header] tab, and edit the items to display in the report.**




**4** **Click the [Scale/Title/Range] tab.**




1 Deselect [Auto] for the X-axis (wavelength) and Y-axis (intensity) in the [Display Area], and enter the desired scale.

2 To output reports of lambda max or lambda min spectrum, select [Lambda max Label] or [Lambda min Label], and click [Format].

**5** **Click [OK].**

**Reference**

Refer to *"5.7.4 Preview Before Printing" P.172* for details.

## ■ Change the Content and Print Scale for Library Search Results

Use the pre-installed report format file “PDADataAnalysisResults.lsr” to print library search results. Refer to *"5.7.2 Open Report Format Files"* to open “PDADataAnalysisResults.lsr”.

**NOTE**

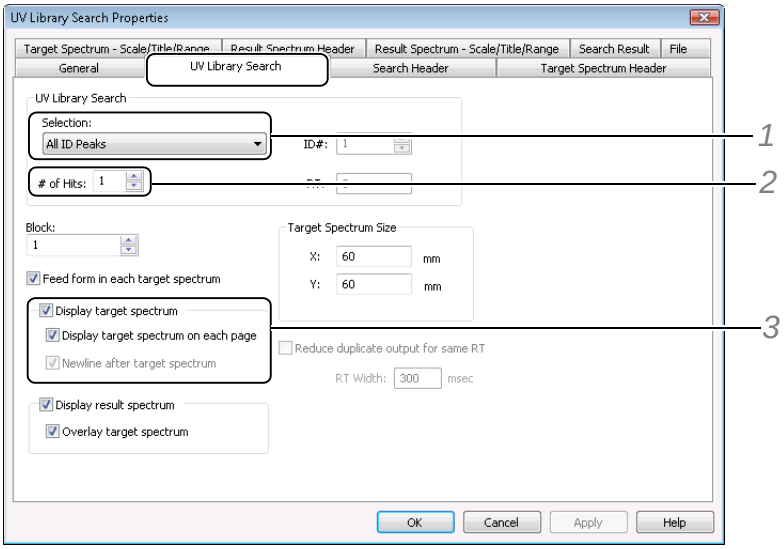
Data processing parameter changes on the [Library Search] tab for the data file are not printed even if the library search results are printed. Add the [Method] item to print the settings made on the [Library Search] tab.

**1** **Double-click the [UV Library Search] item.**

**NOTE**

The [UV Library Search] item is located on the second page of “PDADataAnalysisResults.lsr”.

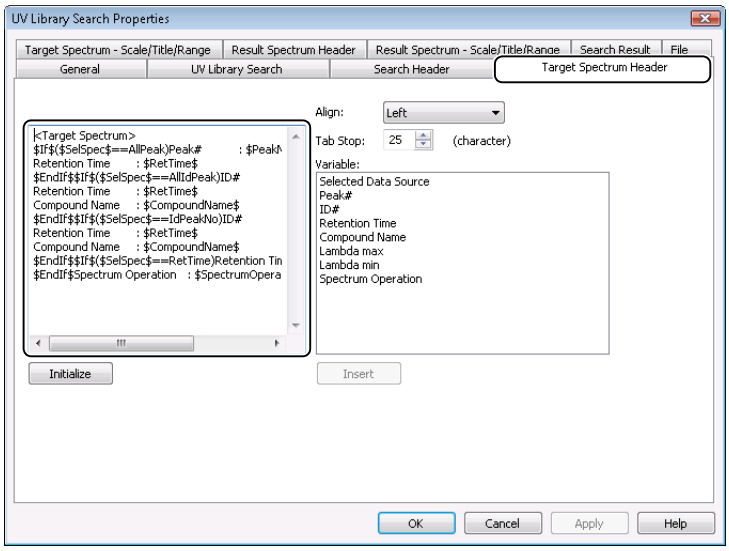
**2** **Click the [UV Library Search] tab.**




*1* Select the searched peaks to display in the [Selection] list.
*2* Enter the number of hits to display at [# of Hits].
*3* Select the target spectrum print method at [Display target spectrum].

**3** **Click each of the [Search Header], [Result Spectrum Header], and [Target Spectrum Header] tabs, and edit the header information to display in the report.**

The [Target Spectrum Header] tab is shown in the following example.

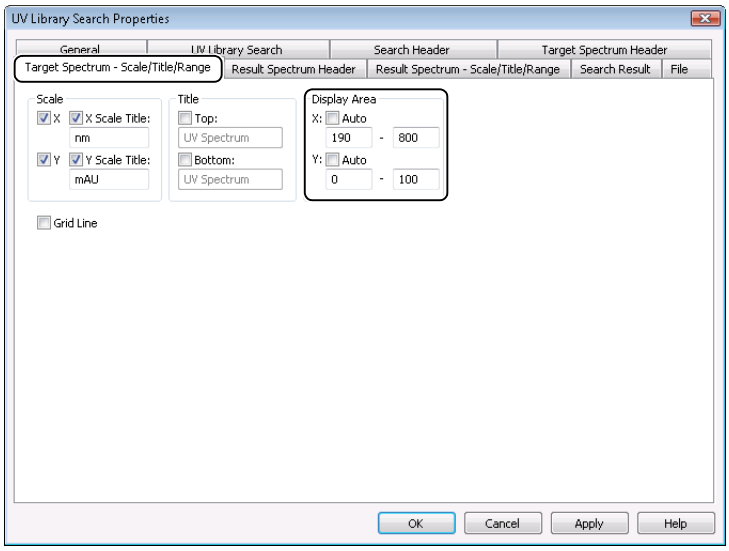



**Reference**

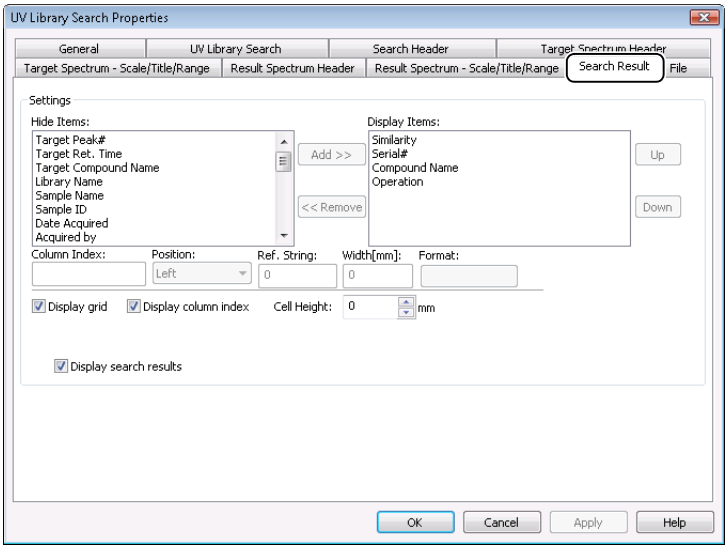
Refer to *"7.5.10 Edit Calibration Curve Information" P.267* for more details.

**4** **Click each of the [Result Spectrum - Scale/Title/Range], and [Target Spectrum - Scale/Title/Range] tabs and under [Display Area], deselect [Auto] for X-axis (wavelength) and Y-axis (intensity). Then, enter the desired scale.**

The [Target Spectrum - Scale/Title/Range] tab is shown in the following example.



**5** **Click the [Search Result] tab, and select the table information to be displayed for each of the spectra hit (found) in the search.**




**6** **Click [OK].**

**Reference**

Refer to *"5.7.4 Preview Before Printing" P.172* for details.

## ■ Specify the Peaks and Calculation Method to Print the Peak Purity Calculation Results

Use the pre-installed report format file “PDADataAnalysisResults.lsr” to print peak purity calculation results. Refer to *"5.7.2 Open Report Format Files"* to open “PDADataAnalysisResults.lsr”.

**NOTE**

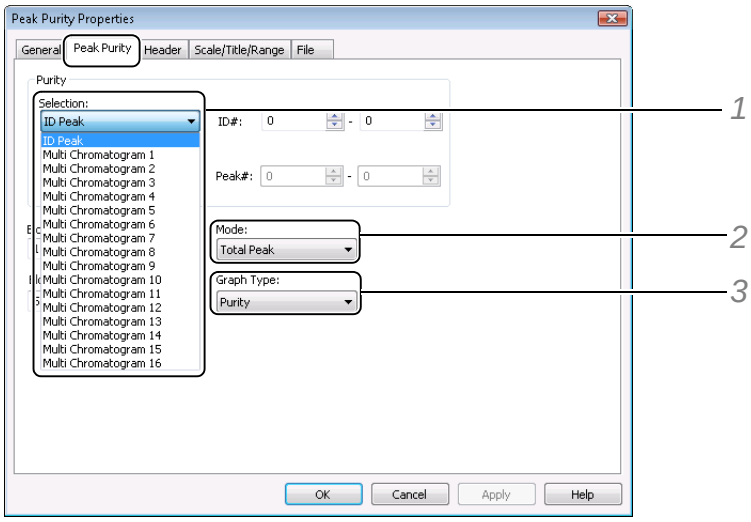
Data processing parameter changes made on the [Purity] tab for the data file are not printed even if the peak purity calculation results are printed. Add the [Method] item to print the settings made on the [Purity] tab.

**1** **Double-click the [Peak Purity] item.**

**NOTE**

The [Peak Purity] item is located on the third page of “PDADataAnalysisResults.lsr”.

## 2 Click the [Peak Purity] tab.




*1* Select the peaks to display in the [Selection] list.

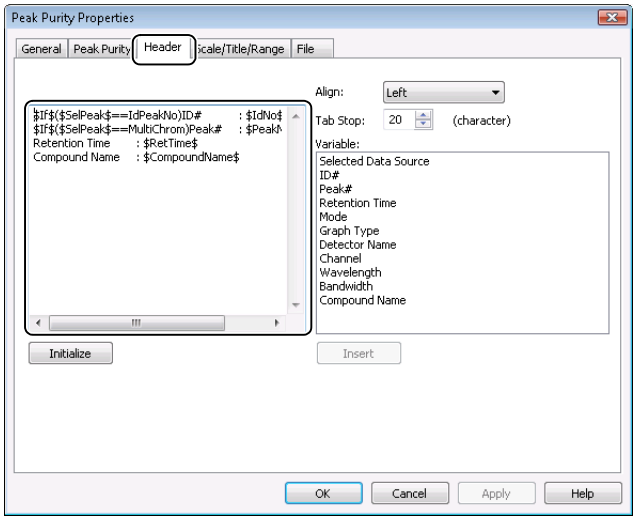
If [ID Peak] is selected, select the calculation results to print by entering the ID#s of the compounds in the Compound Table. The calculation results of all identified peaks are printed if [0]-[0] is entered.

If [Multi Chrom] is selected, select the number of the peak at [Peak #]. The calculation results of all detected peaks are printed if [0]-[0] is entered.

*2* Select the purity calculation mode in the [Mode] list.

*3* Select the display graph in the [Graph Type] list.

## 3 Click the [Header] tab, and edit the items to display in the report.




**Reference**

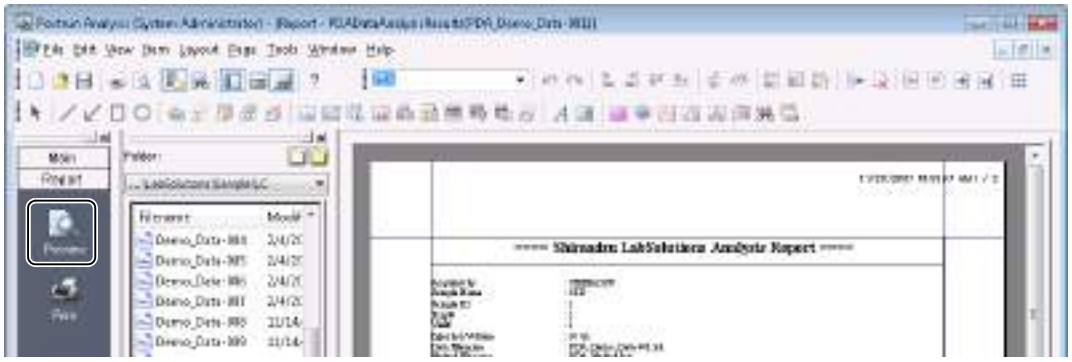
Refer to *"7.5.10 Edit Calibration Curve Information" P.267* for details.

## 4 Click [OK].

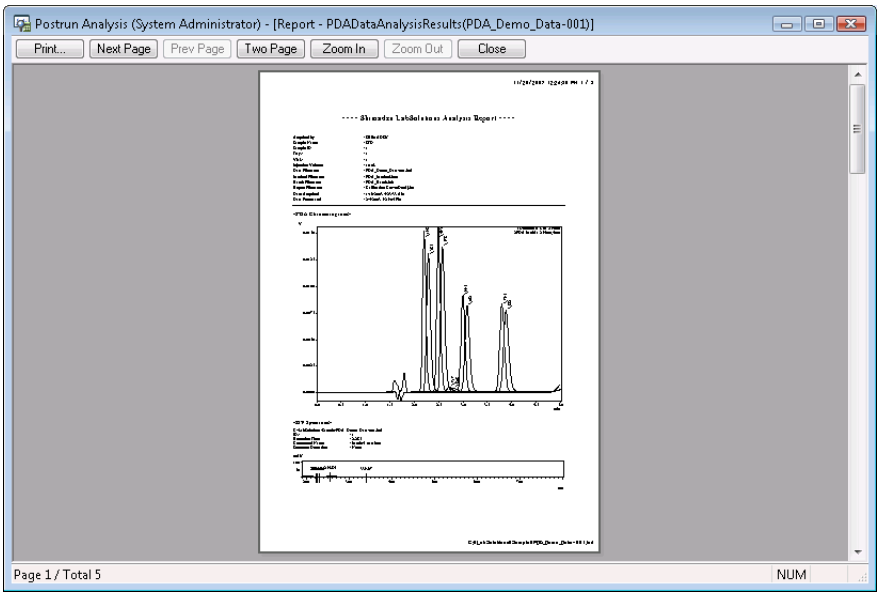
## 5.7.4 Preview Before Printing

Preview the print details set in *"5.7.3 Edit PDA Report Format"* before printing the report.

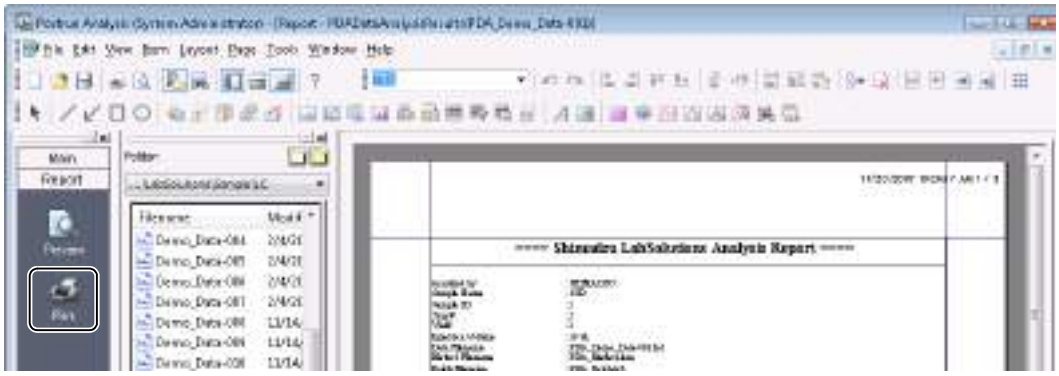
**1** **Click the (Preview) icon on the [Report] assistant bar.**



**2** **Check the report in the preview sub-window, and click [Close].**




**3** **Click the (Print) icon on the [Report] assistant bar.**



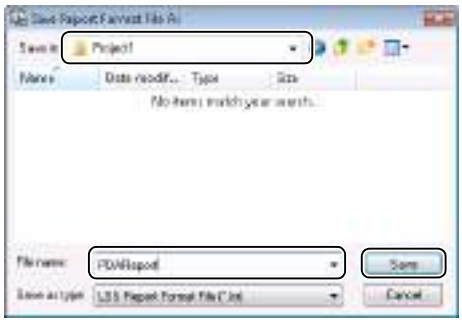
The report is printed.

## 5.7.5 Save Report Format Files

Once a report format is complete, save the report format file under a new name.

**1** **Click [Save Report Format File As] on the [File] menu.**

**2** **Set [Save in], enter the file name, and click [Save].**



# 6 MS Data Analysis

This chapter describes how to acquire data on an MS detector, to display obtained chromatograms and spectra, and set data processing parameters during postrun analysis.

Qualitative and quantitative processing is performed on compounds in unknown samples. In qualitative processing, peak integration is performed on chromatograms to detect peaks and search for obtained spectra in a library. In quantitative processing, the concentration of compounds in an unknown sample is calculated according to a calibration curve created form a standard sample of a known concentration.

## 6.1 [MS Data Analysis] Window

The [MS Data Analysis] window is comprised the following sections.

- [Chromatogram View] - displays chromatograms
- [Spectrum View] - displays spectra
- [Results View] - displays Peak Tables and quantitative results
- [Method View] - displays data processing parameters

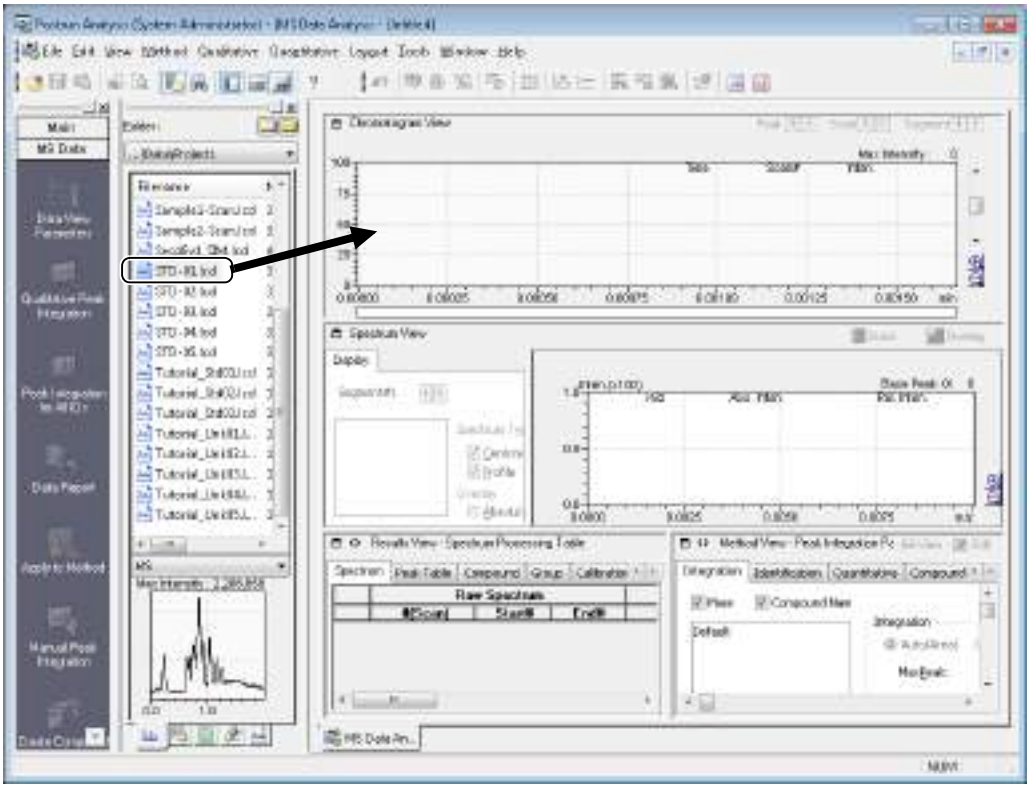


### 6.1.1 Open the [MS Data Analysis] Window

**1** **Click the**  **icon in the [LabSolutions Main] window, and double-click the [Postrun] icon.**

**2** **Click the (MS Data Analysis) icon on the [Main] assistant bar in the [Postrun Analysis] program.**

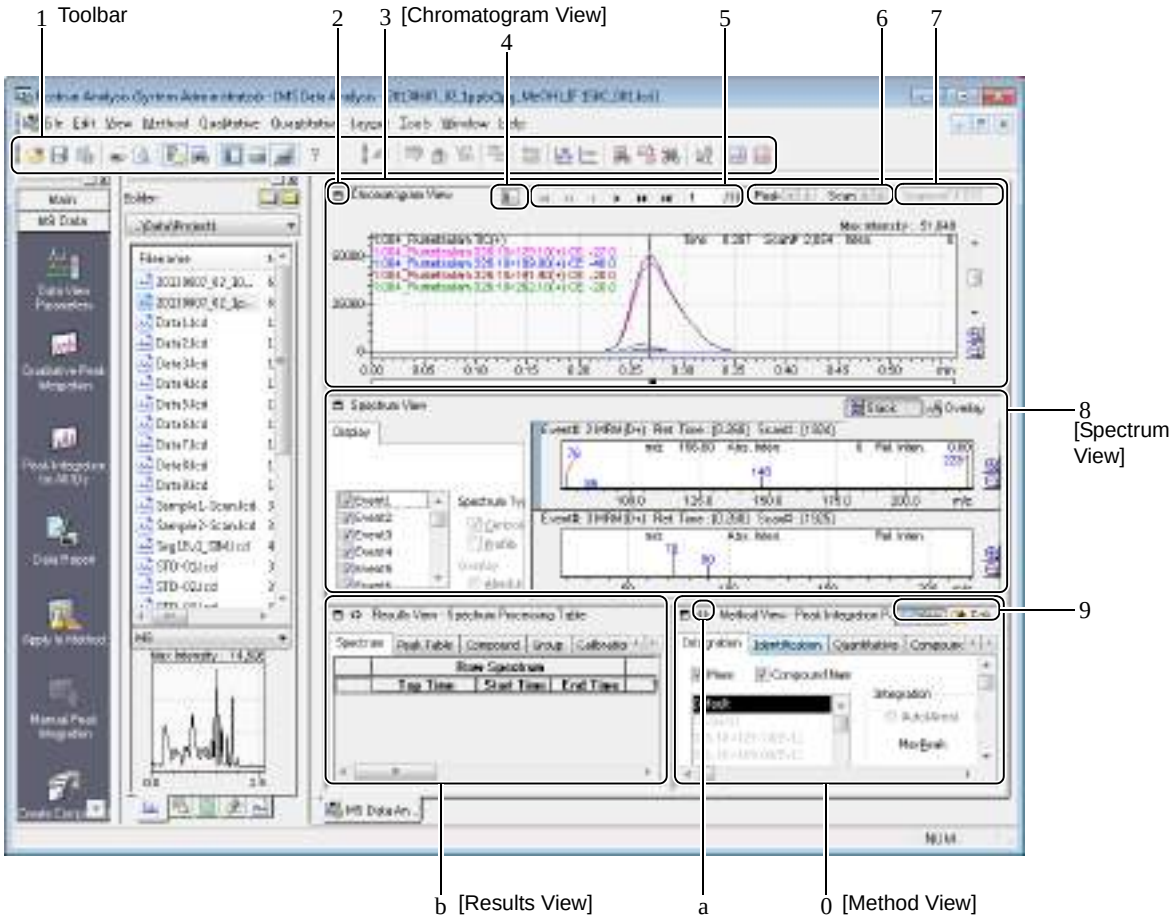
**3** **Drag-and-drop the MS data file onto the [MS Data Analysis] window from the [Data Explorer] sub-window.**



The contents of the data file are displayed in the [MS Data Analysis] window.

## 6.1.2 [MS Data Analysis] Window Description

This section describes how to view and use the [MS Data Analysis] window.

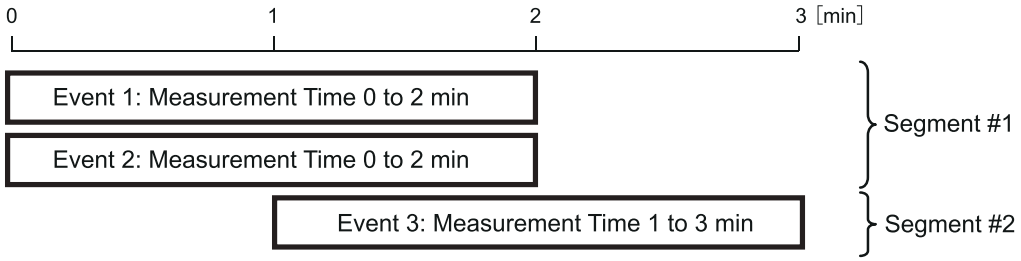



| No. | Explanation |
|---|---|
| 1 | Displays the [Standard] and [MS Data Analysis] toolbars. |
| 2 | Click this icon in each sub-window to expand the sub-window to a full-screen view and again to return the view back to the normal size view. |
| 3 | Displays the chromatograms in the open data file. Double-click on a chromatogram to display the spectrum extraction line (vertical cursor). The [Spectrum Process Bar] displayed at the bottom shows the range where the spectrum underwent average/subtraction processing.<br>Refer to *"6.2.8 Manual Average/Subtraction Processing on Spectra" P.194* for details on average/subtraction processing of spectra. |
| 4 | The chromatogram line width displayed in the [Chromatogram View] can be emphasized.<br>**NOTE**<br>This item can be chosen, when display modes are [View All Segments] and [View Multiple Segments], or when it is in [Overlay] mode at the time of [View Each Segment]. |
| 5 | Allows changing the active block.<br>The number of blocks to be displayed in a single window and the number of chromatograms to be displayed in one block are specified on the [Chromatogram Table] tab in the [MS Data View Parameters] sub-window. |
| 6 | Moves the spectrum extraction line on the chromatogram. Click the [Peak] button to move the spectrum extraction line moves to the next peak top. Click the [Scan] button to move the spectrum extraction line in small increments. |
| 7 | Click the [Segment] button to change the displayed segment when [Chromatogram View] is set to [Each Segment]. Refer to *"6.2.4 Change the [Chromatogram View] Display Mode" P.183* for details on [Each Segment]. |
| 8 | Displays the MS spectrum at the time selected by the spectrum extraction line on the chromatogram. |

| No. | Explanation |
|---|---|
| 9 | Click Edit (Edit Mode) to change the data processing parameters in the method. Click View (View Mode) after editing the parameters to reflect the changes in the [Method View]. |
| 0 | Displays the data processing parameters. |
| a | (Wide Size) or (Normal Size) is displayed in [Results View] and [Method View], use them to stretch the sub-windows across the screen in the horizontal direction and return to the normal size display. |
| b | Displays the analysis results. |

**NOTE**

- Files currently being edited in other windows are [Read Only] and cannot be saved. Exit the other application and open the file again to save the results of editing.
- The [MS Data Analysis] window displays the contents of only one data file. Open the [Quant Browser] or [Data Browser] window to check the contents of multiple data files. Refer to *"11 Quant Browser" P.327* or *"12 Data Browser" P.347* for details.
- The [MS Data Analysis] window is comprised of views that are separated by several dividers. The views can be resized by dragging these dividers with the mouse.
- Click [Save Layout] on the [Layout] menu in the [MS Data Analysis] window to save the layouts for each view. Click [Select Layout] on the [Layout] menu in the [MS Data Analysis] window to open a saved layout.
- Click [Layout for Qualitative] or [Layout for Quantitative] on the [Layout] menu in the [MS Data Analysis] window to display the ideal layout for the respective processing type.
- Click [Display All] on the [Layout] menu in the [MS Data Analysis] window to return to the default layout.
- Click [Rollback to Original Data] on the [File] menu return the data processing parameters to those when the data was acquired.
- For data obtained using the MS detector, event groups that have the same measurement starting and ending time are displayed as a segment. In the example shown below, event 1 and event 2 are considered segment #1 and event 3 is segment #2.



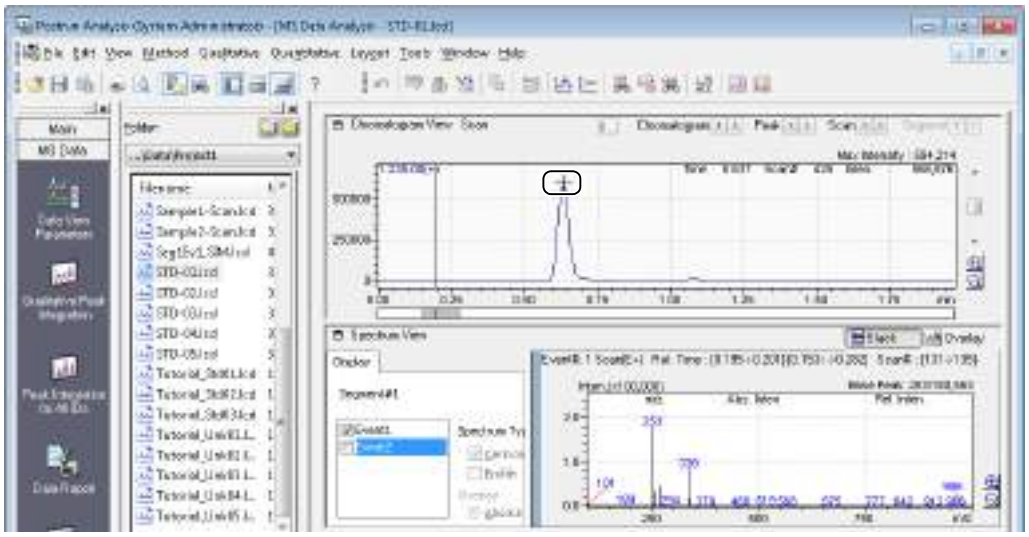
# 6.2 Display Chromatograms and Spectra

This section describes how to display chromatograms and spectra on the [MS Data Analysis] window.

## 6.2.1 Spectra from [Chromatogram View]

Double-click a chromatogram in the [Chromatogram View] to move the spectrum extraction line to that position, and display the spectrum in the [Spectrum View].

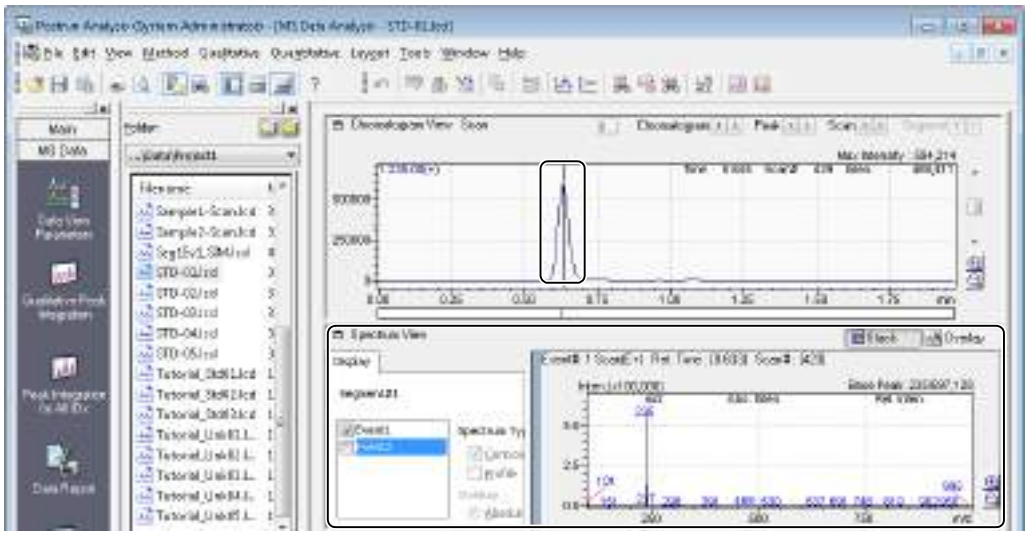
**1** **In the [Chromatogram View], double-click the time to be extracted as the spectrum.**



**NOTE**

If a time is selected within peak detection, the displayed spectrum undergoes average or subtraction processing based on the spectrum processing parameters.

The spectrum extraction line moves, and the spectrum at that time position is displayed in [Spectrum View].



**NOTE**

- Click the [Peak] buttons at the top of the [Chromatogram View] to move the spectrum extraction line to the next peak top (RT). Peaks must already have been detected to use this function.
- The spectrum that is displayed when the [Peak] button is clicked undergoes average/subtraction processing based on the spectrum processing parameters.
- Click the [Scan] button at the top of the [Chromatogram View] to move the spectrum extraction line moves by the preset scan unit.

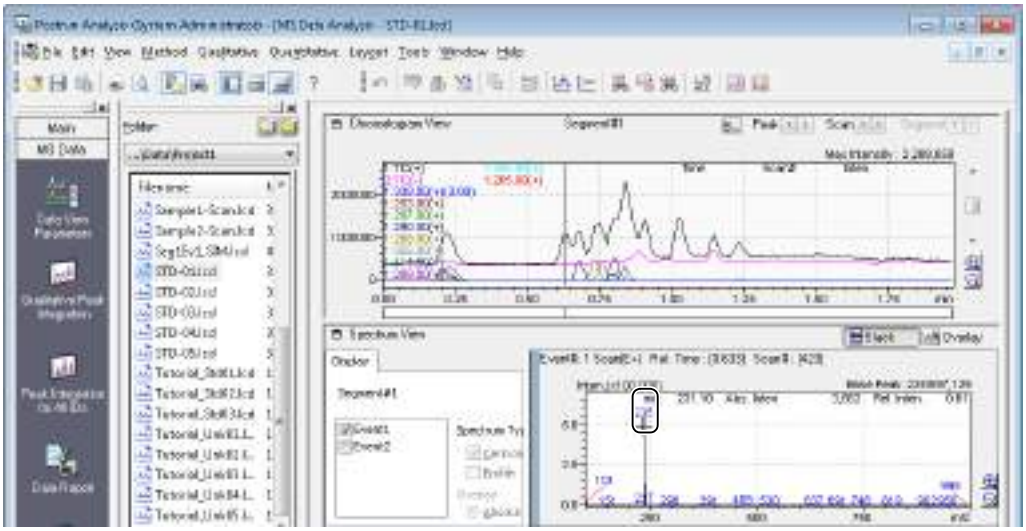
**Reference**

Refer to *"6.3.1 Qualitative Peak Integration" P.199* for details on peak integration and *"6.2.7 Average/Subtraction Processing on Spectra" P.192* for details on spectrum processing parameters.

## 6.2.2 Chromatograms from [Spectrum View]

Double-click a spectrum peak in [Spectrum View] to display the chromatogram of that *m/z* in the [Chromatogram View].

**1 Double-click the *m/z* in [Spectrum View] that is to be extracted as the chromatogram.**



The chromatogram of that *m/z* is listed in the Chromatogram Table and added to the [Chromatogram View].

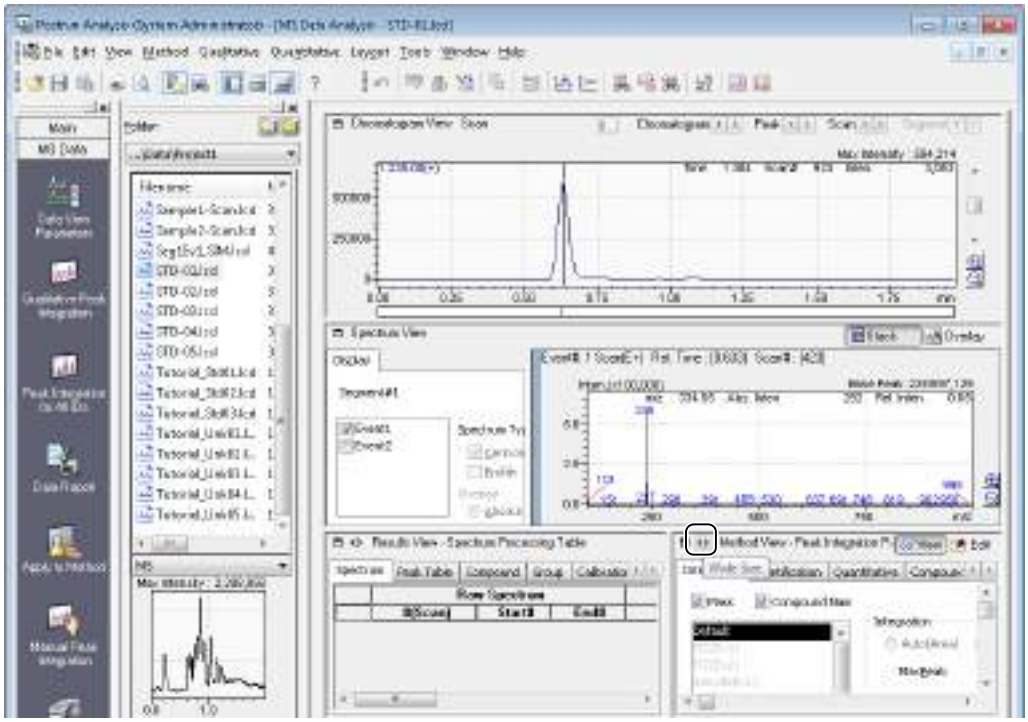
**Reference**

Refer to *"6.2.6 Display Chromatograms from the Chromatogram Table and MIC Table" P.188* for details on the Chromatogram Table.

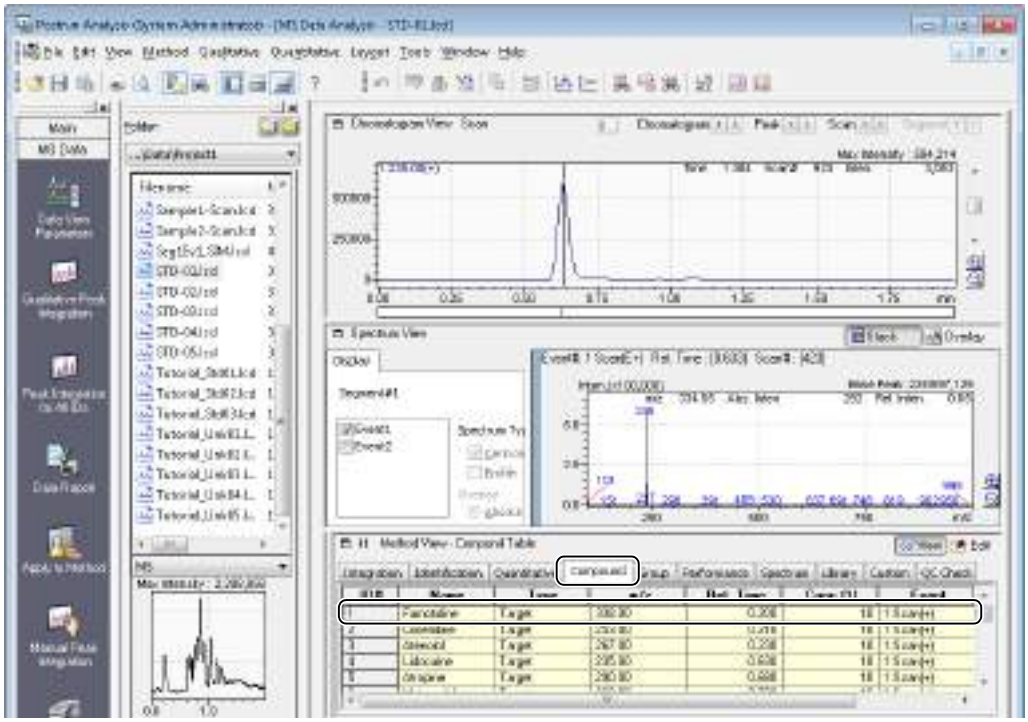
## 6.2.3 Display Chromatograms and Spectra from the Compound Table

Click a row in the Compound Table on the [Compound] tab in [Method View] to display all of the spectra for the time of the identified peak.

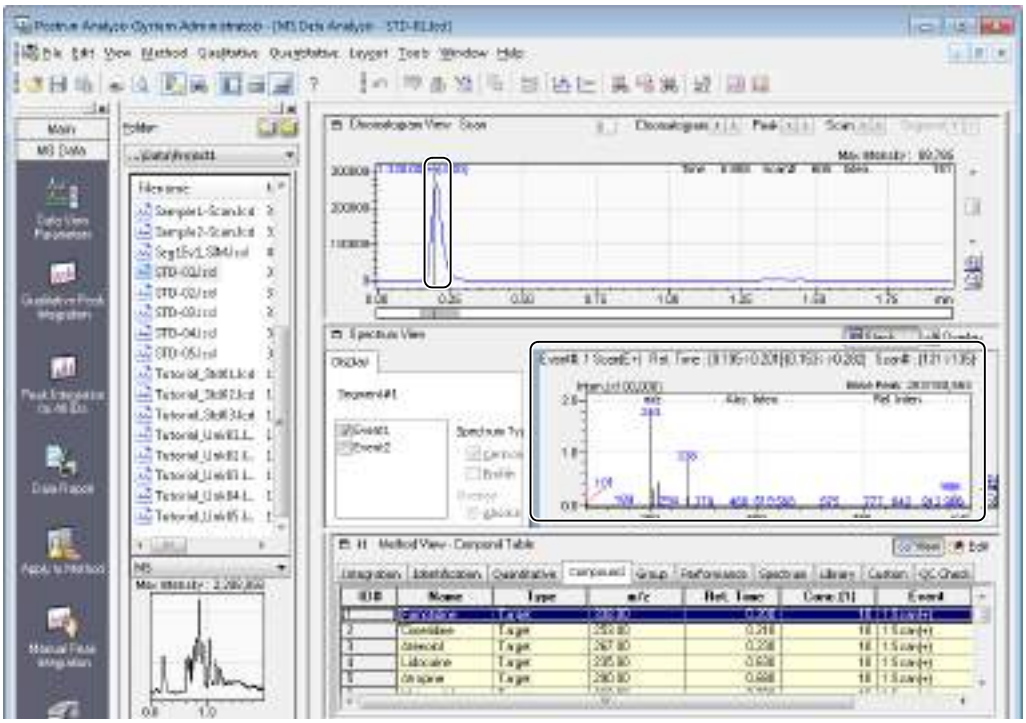
**1** **Click <> (Wide Size) in [Method View].**



**2** **Click the [Compound] tab in [Method View], and click the row of target compound.**



The spectrum extraction line moves to the time position in [Chromatogram View] where that compound is identified, and the spectrum in [Spectrum View] is updated.



## 6.2.4 Change the [Chromatogram View] Display Mode

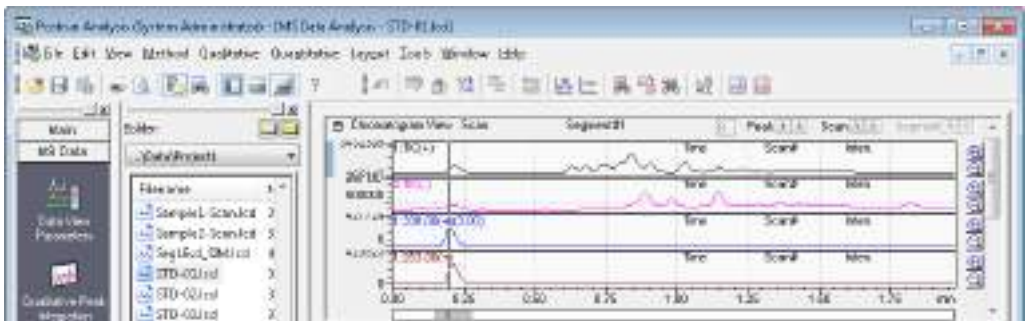
The display in [Chromatogram View] can be changed to [View All Segments], [View Multiple Segments] or [View Each Segment].

In the [View Multiple Segments], segments are displayed in the [Chromatogram View] as blocks containing the specified number of segments. To switch blocks, use the spin button at the top of the [Chromatogram View].

In the [View Each Segment], the chromatogram can be viewed as an [Overlay], [Stack] or [Single] view. This section describes how to change the chromatogram display from [Overlay] to [Stack].

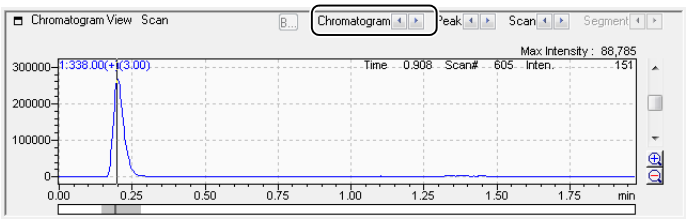
**1** **Right-click on the desired chromatogram in the overlay display and select [View Each Segment], and click [Stack].**


The chromatograms are displayed in a stack and the focus bar is displayed to the left of the active chromatogram.



**NOTE**

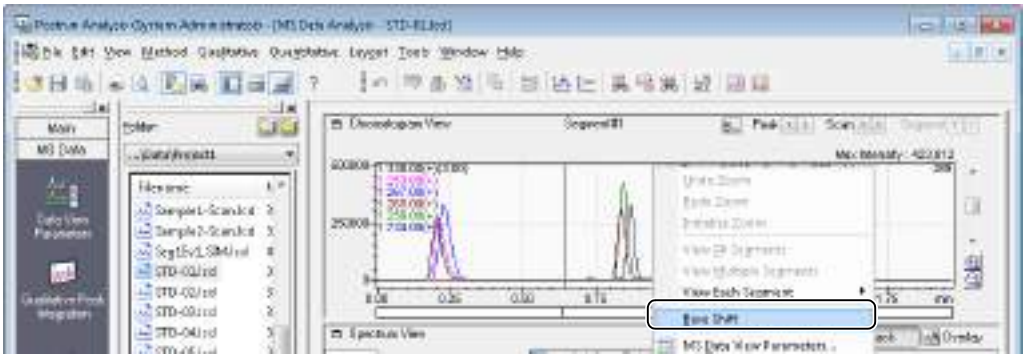
- When [All Segments] is selected, only the [Overlay] setting is available.
- The [Single] setting displays each chromatogram individually. Select the ◀ ▶ at the top of the [Chromatogram View] to change the displayed chromatogram. The ◀ ▶ buttons are only displayed when [Single] is selected.



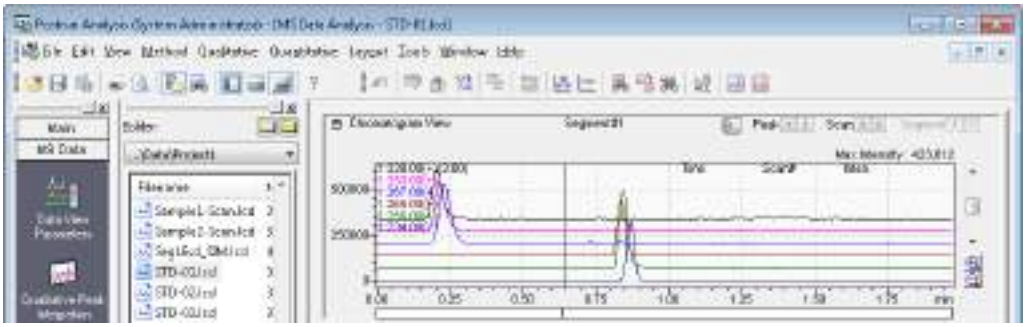
## ■ Display Multiple Chromatograms in the Base Shift View

The base of each chromatogram displayed in the overlay can be shifted to make them easier to identify.

**1** **Right-click on the desired over lay chromatogram, and select [Base Shift].**



The chromatograms are displayed with their bases shifted.

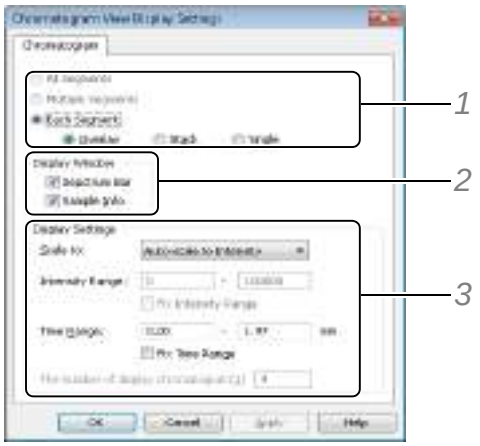


## ■ Chromatogram View Display Settings

Set the chromatogram display mode, whether to display [Spectrum Process Bar] and [Sample Info.], and the chromatogram display range in the [Chromatogram View Display Settings] sub-window.

**1** **Right-click on [Chromatogram View], and click [Display Settings].**

**2** **Select the desired items, and click [OK].**




*1* Select the chromatogram display mode.

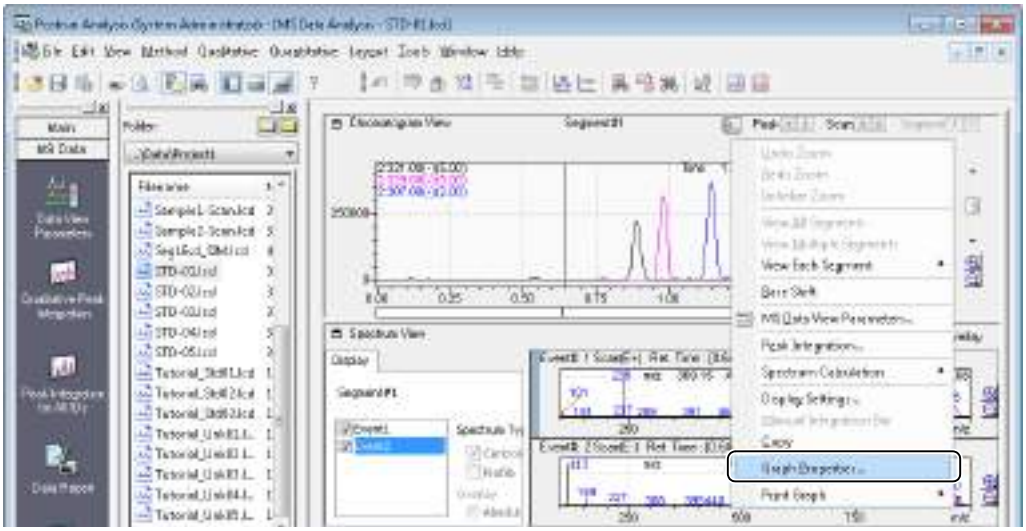
*2* Determine whether to display the [Spectrum Process Bar] and [Sample Info.] in [Chromatogram View].

*3* When [Auto-scan to Intensity] is selected at [Scale to], the intensity axis of the chromatogram is displayed according to the maximum intensity. If [User Defined] is selected, set the range of the intensity axis to display at [Intensity Range].

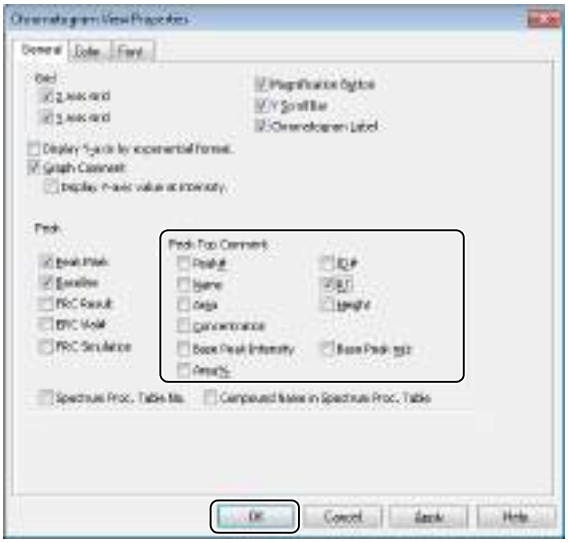
## ■ Peak Top Comments

This section describes how to display the retention time at the top of the peak.

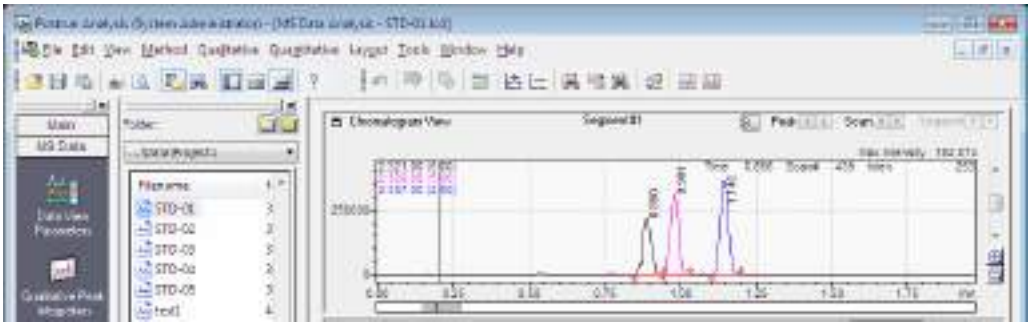
**1** **Right-click on the chromatogram, and then click [Graph Property].**



**2** **Select the peak top comment to display on the chromatogram, and click [OK].**



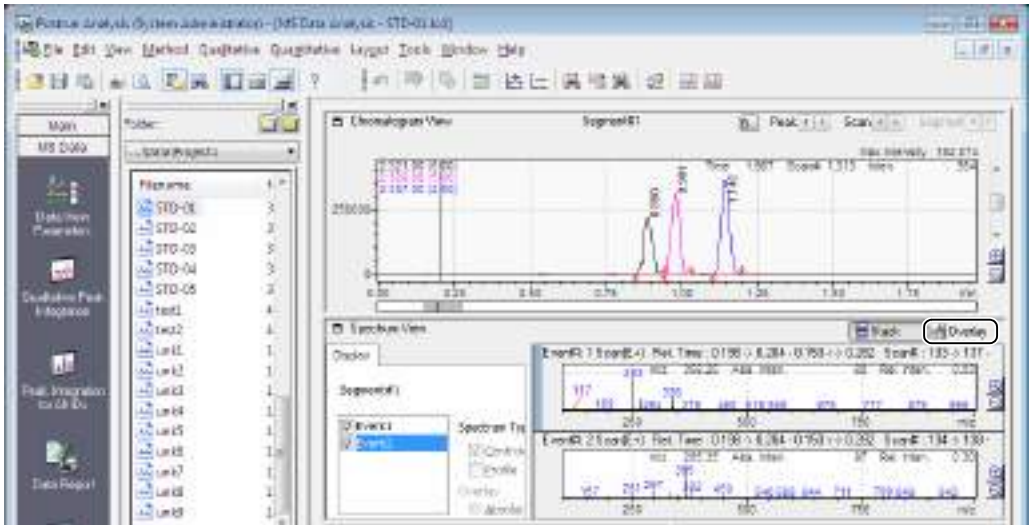
In this example, the retention time is displayed at the top of the peak.



## 6.2.5 Change the [Spectrum View] Display Mode

If the inside of a segment contains multiple events, the spectra acquired for each individual event can be displayed as a stack or an overlay. This section describes how to change from a stack display to an overlay display.

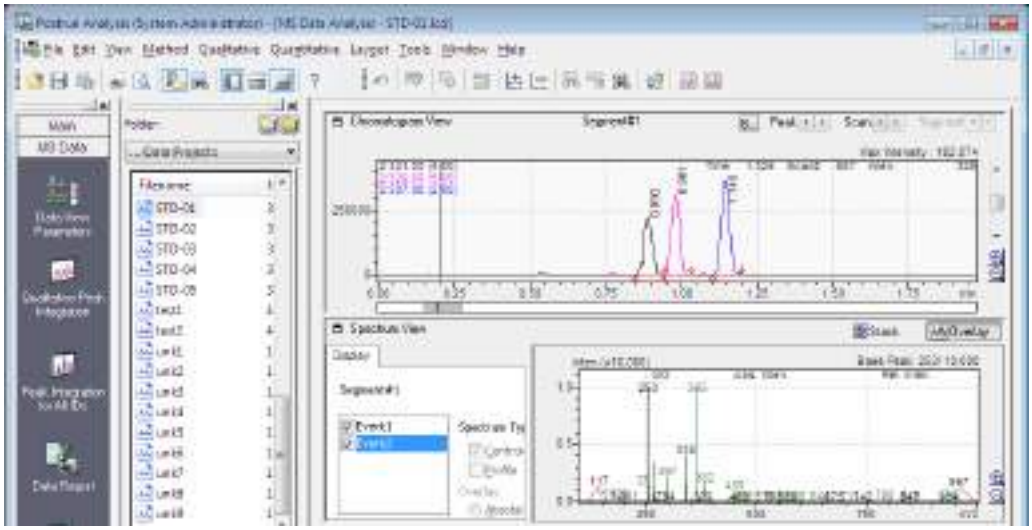
**1** **Open a data file that contains multiple events inside the same segment, and click [Overlay].**



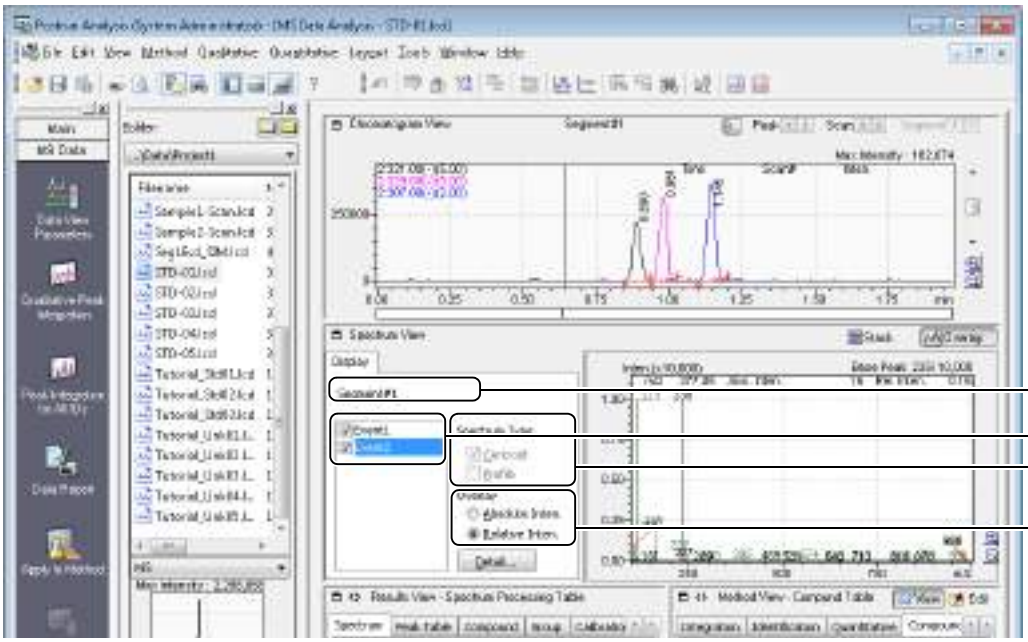
**NOTE**

When multiple spectra are displayed in the stack display mode, the focus bar is displayed to the left of the active spectrum.

All currently displayed spectra are displayed in the overlay display mode.



**2** **Make the desired selections.**




1 If data acquisition was performed with multiple segments, click [◀][▶] to change the displayed segment.

2 Determine whether to display spectra for each event when data acquisition was performed with multiple events.

3 If profile analysis was performed, set the centroid spectrum display and profile spectrum display. When both display modes are selected, both spectra are displayed simultaneously.

4 Select whether to overlay spectra by absolute intensity or relative intensity.

## 6.2.6 Display Chromatograms from the Chromatogram Table and MIC Table

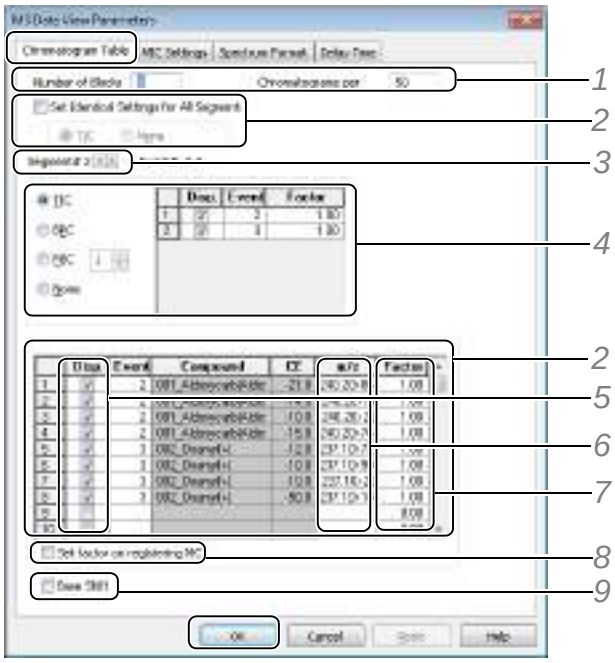
Chromatogram Table and MIC Tables are used to display chromatograms at a specified *m/z* or to display chromatograms that cannot be specified by a single *m/z*, such as TIC/MIC.

### ■ Register Chromatograms in the Chromatogram Table

TIC/MIC selection, MS chromatogram display and base shift are set in the Chromatogram Table. This section describes how to enter the *m/z* and display chromatograms.

**1** **Click the  (Data View Parameters) icon on the [MS Data] assistant bar.**

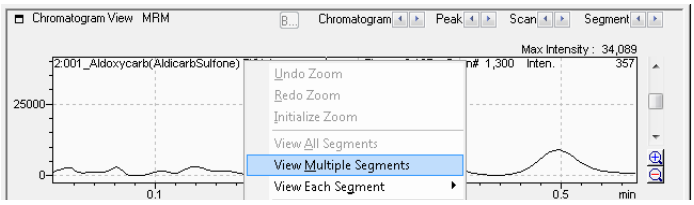
## 2 Click the [Chromatogram Table] tab, set each item, and click [OK].




*1* If the [View Multiple Segments] is selected, sets the number of blocks to be displayed in one window and the number of chromatograms to be plotted per block.

**NOTE**

To select the [View Multiple Segments], attach the checkmark to [View Multiple Segments] on the right-click menu in the [Chromatogram View].




*2* If the [Set Identical Settings for All Segments] is selected, TIC/BPC/MIC/None settings specified for individual segments or events are ignored. And Select [TIC] or [None].

TIC: Specifies using the TIC/MIC mass table for TIC.

None: Ignores TIC/MIS mass table settings and does not display TICs, BPCs, or MICs.

*3* If data acquisition was performed with multiple segments, click to change the target segment.

*4* Specify TIC, BPC or MIC.

Use the table on the right to select the chromatogram to display for each event and the display scale for the intensity axis.

*5* If [Disp.] is selected, the chromatogram for the preset *m/z* is displayed.

*6* Enter the *m/z*.

In this example, enter “338.00” at [m/z].

**NOTE**

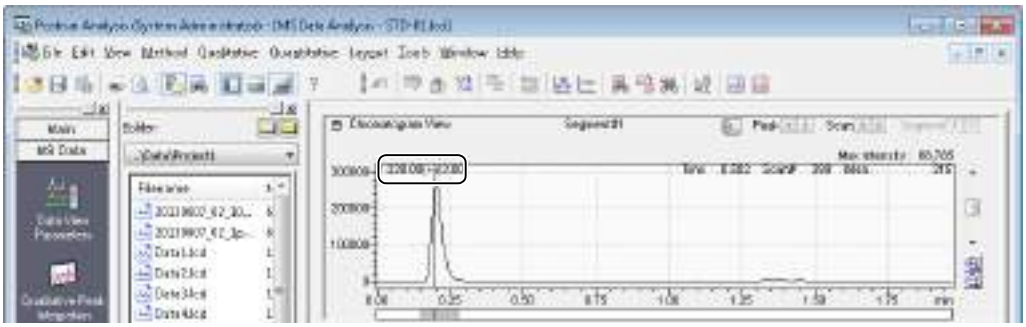
- Enter the [m/z] start and end points delimited with a hyphen to display chromatograms in a specified *m/z* range. (example: 183.00-185.00)
- When displaying chromatograms for MRM events, the [Precursor m/z] and [Product m/z] values separated by a " > " symbol is displayed in a dropdown list box at [m/z]. (Example: 231.10 > 189.00)

*7* Specify the display scale for the intensity axis.

8 If [Spectrum View] is double-clicked and *m/z* is registered to the Chromatogram Table, the scale can be set so that the chromatogram automatically becomes about 50% of the maximum intensity of TIC when [Set factor on registering MC] is selected.

9 Select [Base Shift] to display the chromatogram with its base shifted.

Chromatograms are added to [Chromatogram View] according to the settings made to each item.

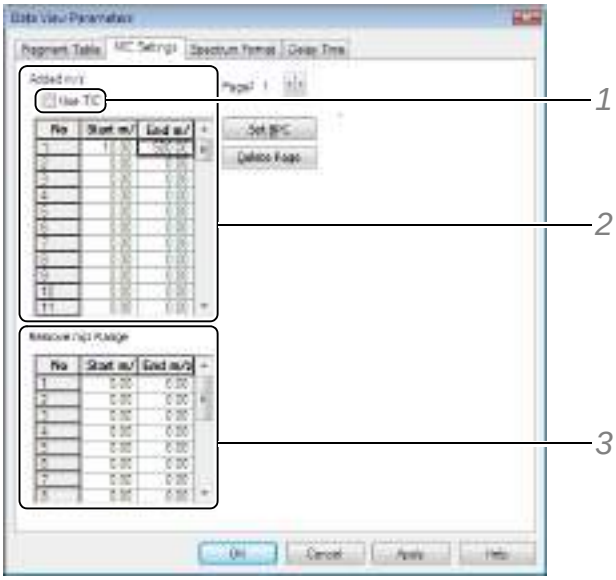


## ■ Edit the MIC Table and Display MIC in [Chromatogram View]

Set the *m/z* range to be integrated in the MIC Table to display MIC in [Chromatogram View].

**1 Click the (Data View Parameters) icon on the [MS Data] assistant bar.**

**2 Click the [MIC Table] tab, and set each item.**




1 Select [Use TIC] so that TIC is used instead of MIC.
Usually, TIC is combined with [Remove m/z Range].

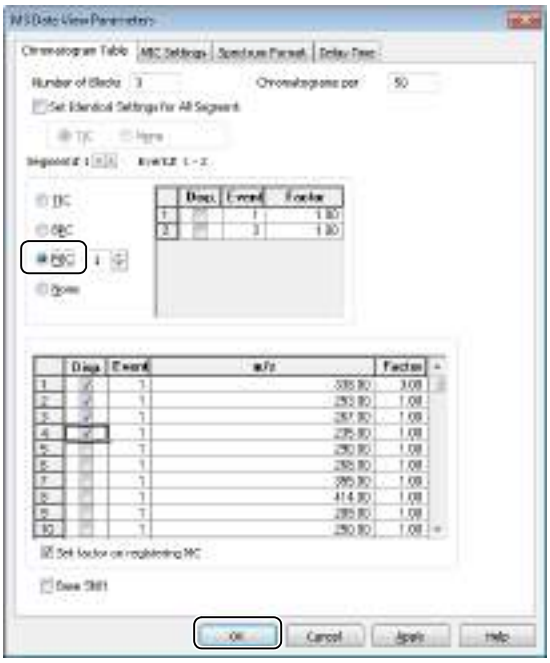
2 Set the *m/z* range of MIC to be integrated.

In this example, change the setting from “10.00” to “500.00”.

3 Set the *m/z* range to exclude from the *m/z* that was set at [Added m/z Range].

- Up to 8 pages can be set. Click [◀][▶] to change the page.
- Click [Delete Page] to delete the contents of the currently displayed [Page #].

## 3 Click the [Chromatogram Table] tab, select [MIC], and click [OK].



The chromatogram obtained by integrating signals within the *m/z* range is displayed in [Chromatogram View].

**NOTE**

The page number can be changed using the box to the right of [MIC] in the Chromatogram Table.

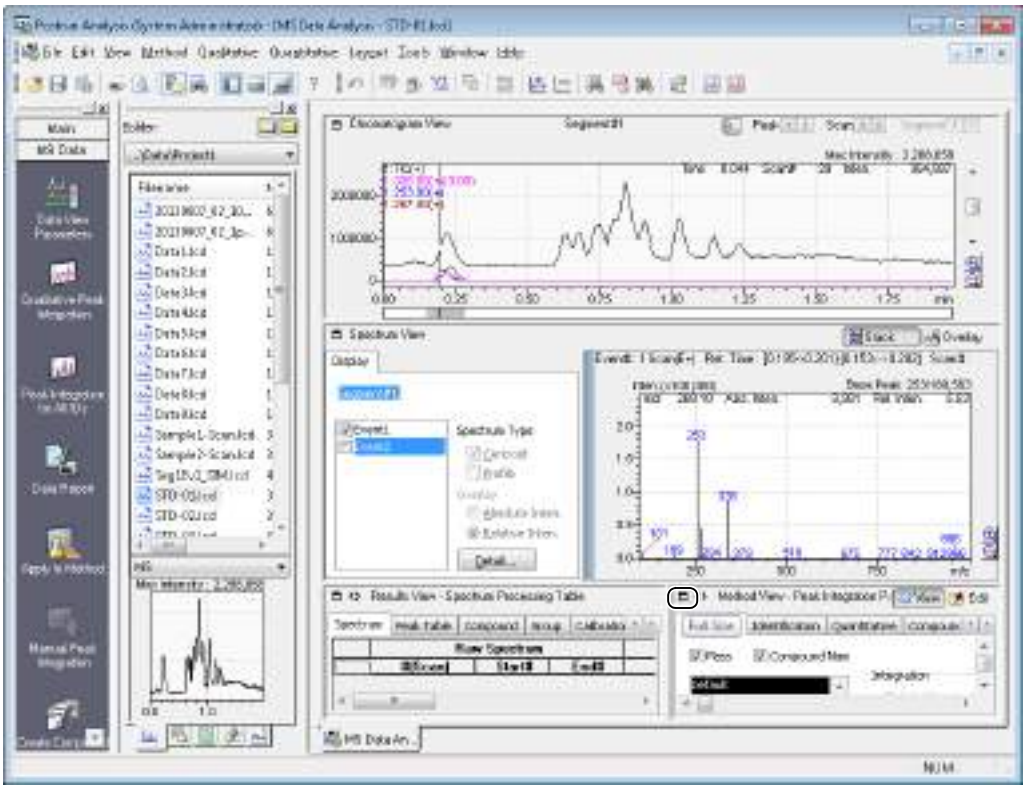
## 6.2.7 Average/Subtraction Processing on Spectra

When a peak is selected and its spectrum is displayed in [Chromatogram View], average/subtraction processing is performed on the spectrum according to the spectrum processing parameters.

### Reference

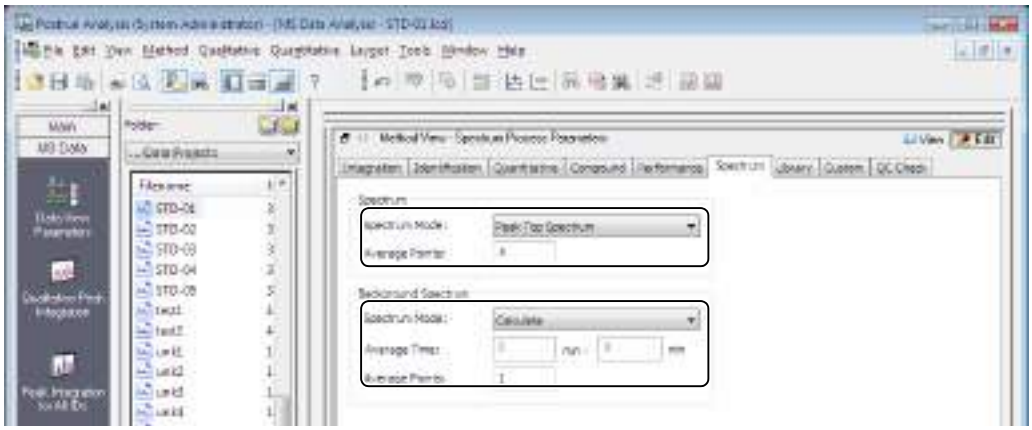
Refer to *"6.2.8 Manual Average/Subtraction Processing on Spectra" P.194* for details on performing manual average/subtraction processing on spectra.

**1** **Click (Full Size) in [Method View].**



**2** **Click Edit (Edit Mode) in [Method View].**

**3** **Click the [Spectrum] tab, and set each item.**



1. When a peak is selected on a chromatogram, select whether to set the displayed spectrum as the peak top (+ number of average points) or to set the displayed spectrum as a spectrum obtained by integrating from the peak start to peak end range.
2. Select the spectrum to be integrated in background.

**4** **Click View (View Mode) in [Method View], and click (Normal Size).**

When the peak is extracted from the chromatogram, the spectrum is processed using the preset conditions.

## 6.2.8 Manual Average/Subtraction Processing on Spectra

Average the spectrum in [Chromatogram View] to obtain an integrated spectrum on any specified time range. Also, subtract spectrum in [Chromatogram View] when performing background processing.

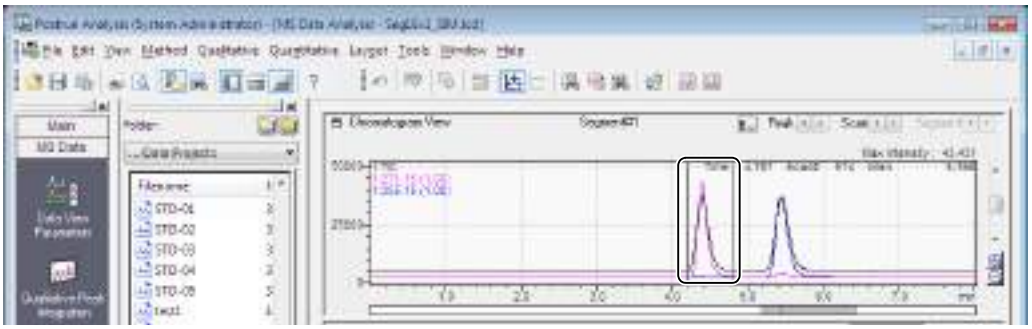
### ■ Average MS Spectra

**1** **Click (Average Spectrum) on the toolbar.**

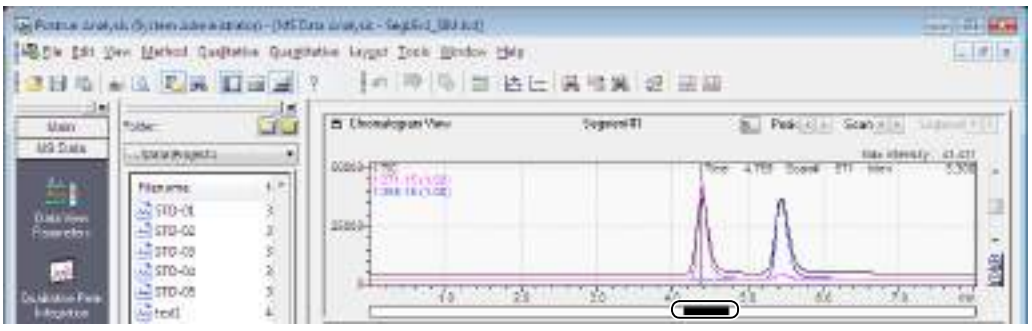
**NOTE**

Spectra can also be averaged by right-clicking on [Chromatogram View], selecting [Spectrum Calculation], and clicking [Average].

**2** **Use the mouse to select the time range to be averaged on [Chromatogram View].**

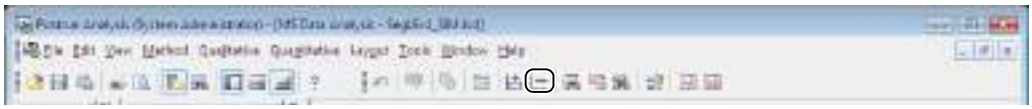


The spectrum averaged within the selected time range is displayed in [Spectrum View].
The averaged time range is displayed in black in [Spectrum Process Bar] at the bottom of [Chromatogram View].



## ■ Subtract MS Spectra

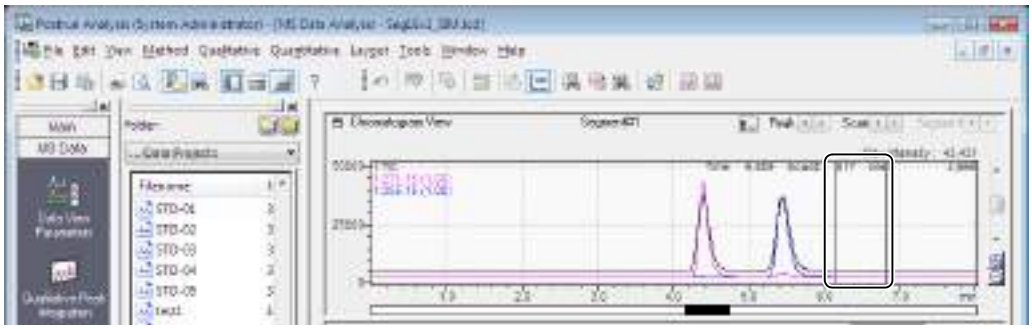
**1** **Click (Subtract Spectrum) on the [MS Data Analysis] toolbar.**



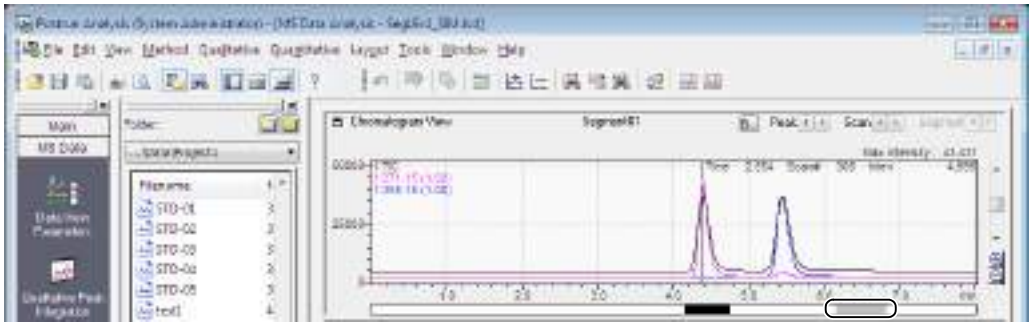
**NOTE**

Spectra can also be subtracted by right-clicking on [Chromatogram View], selecting [Spectrum Calculation], and clicking [Subtract].

**2** **Use the mouse to select the time range to be subtracted on [Chromatogram View].**



The spectrum obtained by subtracting the spectrum in the specified time range in background is displayed in [Spectrum View]. The time range averaged for subtraction is displayed in gray in [Spectrum Process Bar] at the bottom of [Chromatogram View].

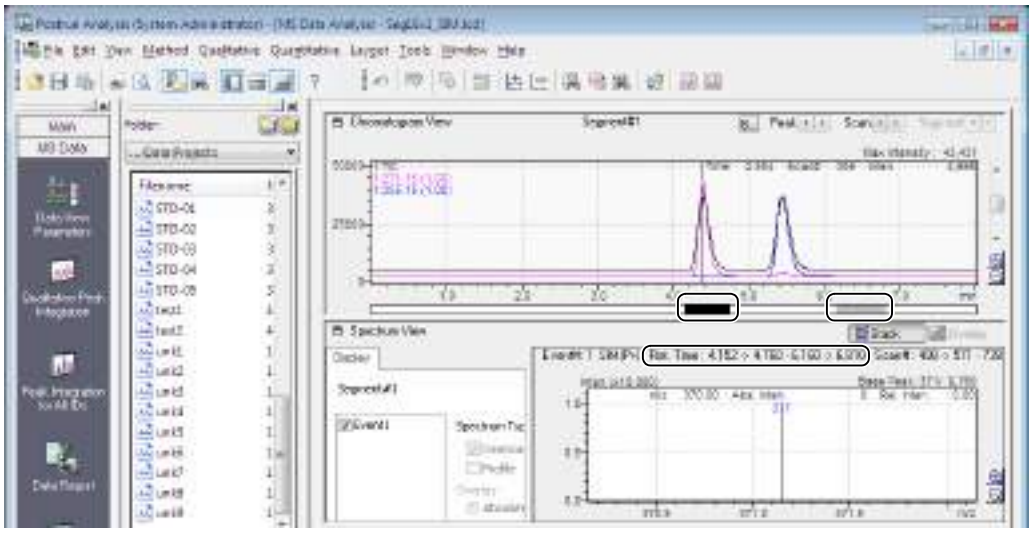


**NOTE**

**Click** (Subtract Spectrum) and double-click the target time in the chromatogram to perform the subtraction process on the spectrum.

### ■ Check Averaged and Subtracted Retention Times in [Spectrum View]

The spectrum-calculated time is displayed at the top of the [Spectrum View]. The following is an example of a subtracted spectrum created by averaging the time 6.160 min to 6.810 min from the spectrum created by averaging the time 4.152 min to 4.760 min.



## 6.2.9 Add Spectra to the Spectrum Process Table

The spectrum displayed in the [Spectrum View] can be entered into the Spectrum Process Table. Processed spectra can be displayed by selecting averaged or subtracted spectra that was previously added to the Spectrum Process Table. Spectra in the Spectrum Process Table are used in reports and library searches.

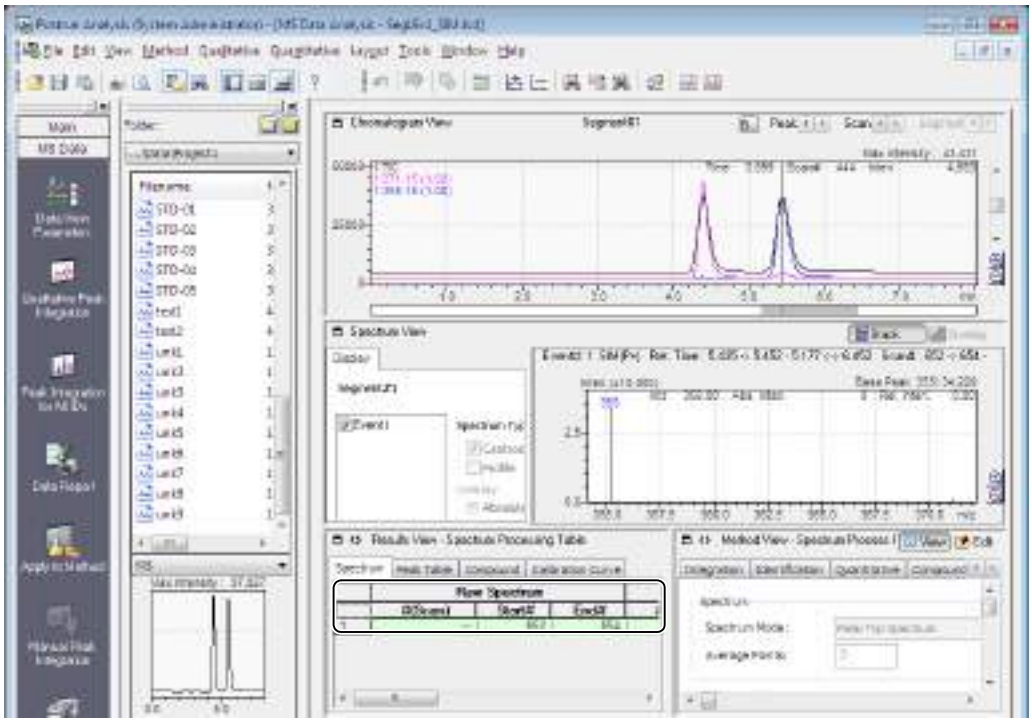
**1** **Display the spectrum in the [Spectrum View], and click (Register to Spectrum Process Table) on the toolbar.**

**NOTE**

Spectra can also be registered by right-clicking on the spectrum display area of [Spectrum View], and clicking [Register to Spectrum Process Table] on the displayed menu.

**2** **Click [OK].**

The spectrum is registered to the Spectrum Process Table on the [Spectrum] tab in [Results View].





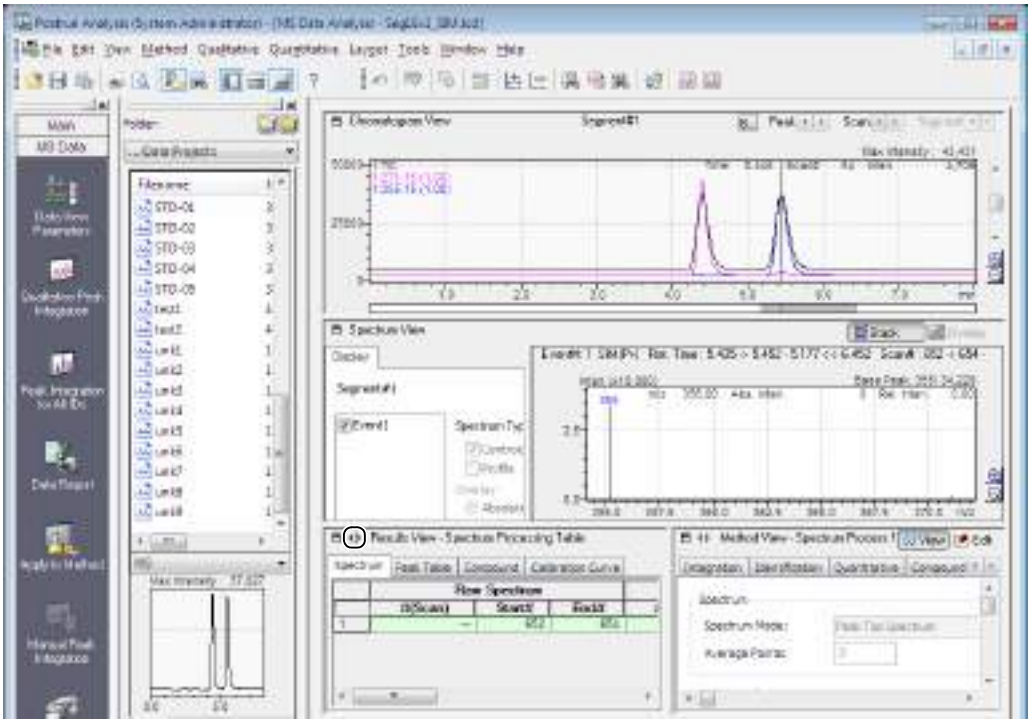
**NOTE**

- Select a row in the Spectrum Process Table to display that information in the [Spectrum View].
- To delete a spectrum, right-click on the Spectrum Process Table, and click [Delete Row] or [Delete Table].

## ■ Sort the Spectrum Process Table by #(Scan) or Top Time (Retention Time)

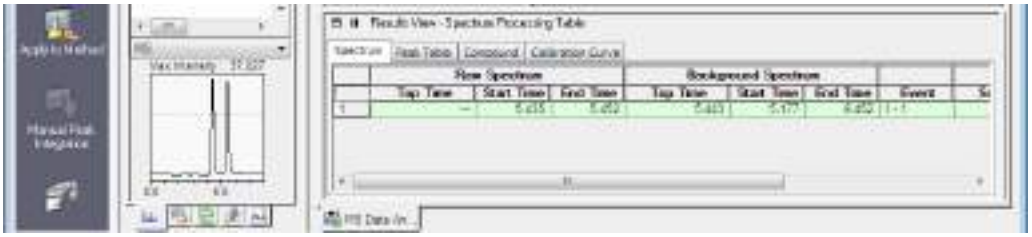
This section describes how to change the sort procedure for the Spectrum Process Table from [#(Scan)] to [Top Time] (retention time).

**1** **Click (Wide Size) in [Results View].**



**2** **Right-click on [#(Scan)] in the Spectrum Process Table, and click [Retention Time].**

[Top Time] (retention time) is displayed in the Spectrum Process Table.



**3** **Click (Normal Size) in [Results View].**

# 6.3 Qualitative Processing

This section describes how to set qualitative peak integration parameters. The chromatogram displayed in [Chromatogram View] is targeted for qualitative processing. The result is displayed in the Spectrum Process Table on the [Spectrum] tab in [Results View] and on the [Peak Table] tab.

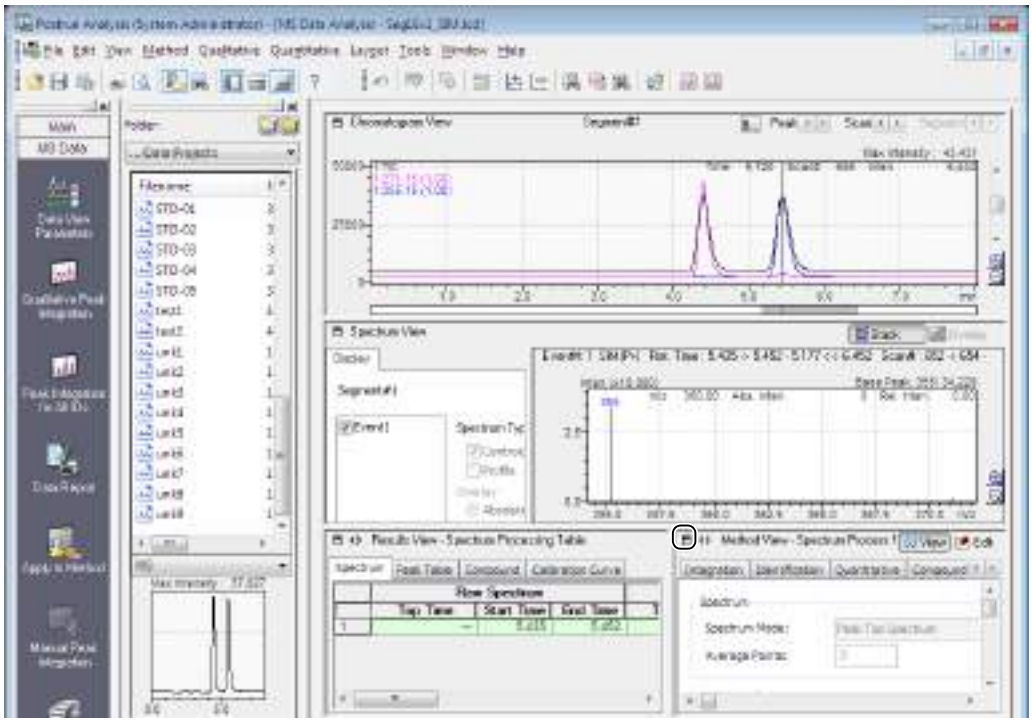
## 6.3.1 Qualitative Peak Integration

This section describes how to set qualitative peak integration parameters in the [Method View].

**NOTE**

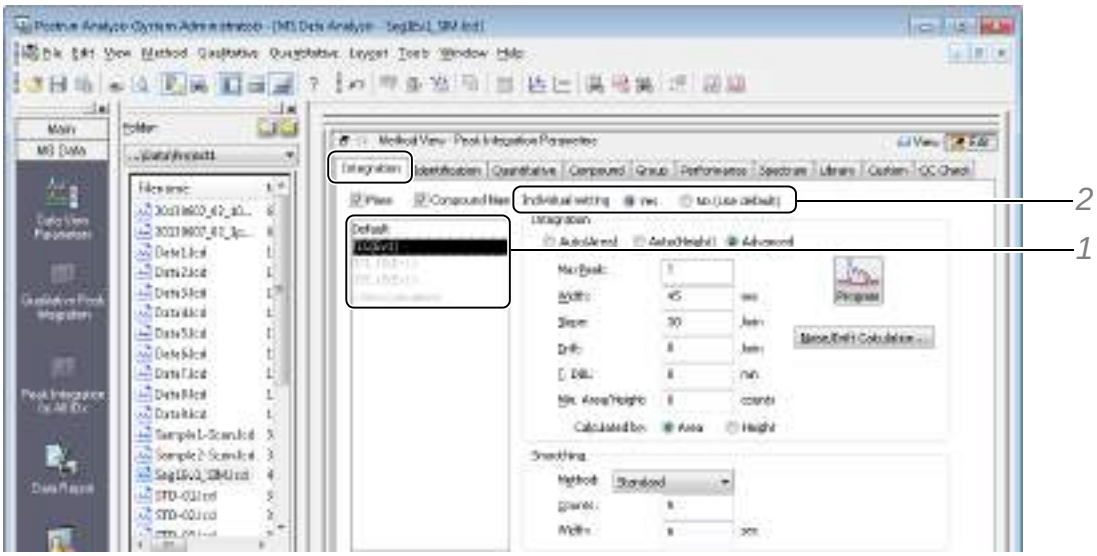
The data processing parameters for the data file displayed in the [MS Data Analysis] window can be edited. The data processing parameters must be saved as a method file before they can be used to process other data files. Refer to the Data Acquisition & Processing Theory Guide for details on the method information stored in the data files.

**1** **Click (Full Size) in [Method View].**



**2** **Click Edit (Edit Mode) in [Method View].**

## 3 Click the [Integration] tab, and set each parameter as required.




1 Select the m/s or compound name from the list and enter the individual peak integration parameters.
Only [Default] and compounds with [Yes] selected at [Individual setting] can be edited.

2 Select whether to set peak integration parameters individually.
Select [No (Use Default)] to perform peak integration using the parameters set as [Default] in the list.

### NOTE

- Click  and enter the integration time program to change peak integration parameters at different times throughout the chromatogram.
- Click [Noise/Drift Calculation], and enter the [Noise/Drift Calculation Settings] parameters to select the method of noise and drift calculation, and the detection and quantitative limit coefficient.
- Right-click on [Method View] and click [Cancel Edit] to cancel editing in [Method View].

**Reference**

Refer to the Data Acquisition & Processing Theory Guide for details on each of the parameters.

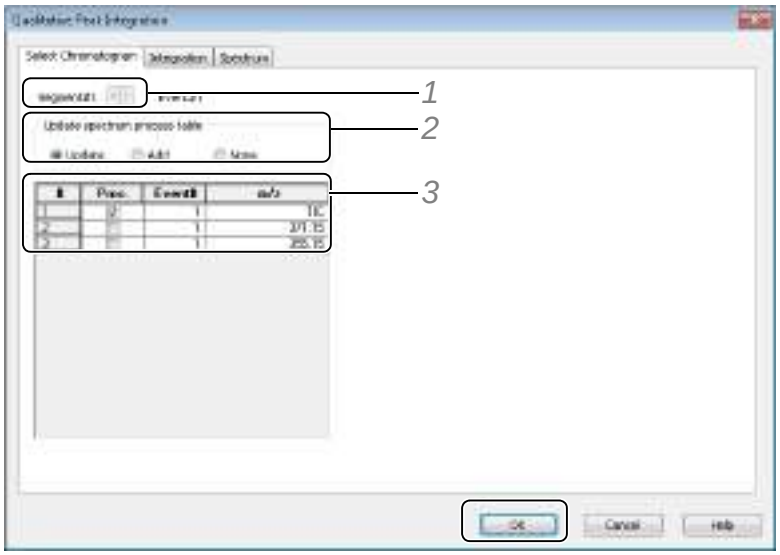
## 4 Click View (View Mode) in [Method View], and then click (Normal Size).

## 5 Click the (Qualitative Peak Integration) icon on the [MS Data] assistant bar.

**NOTE**

The same processing can be achieved by right-clicking on [Chromatogram View] and clicking [Peak Integration].

## 6 Set the parameters in the [Qualitative Peak Integration] sub-window, and click [OK].

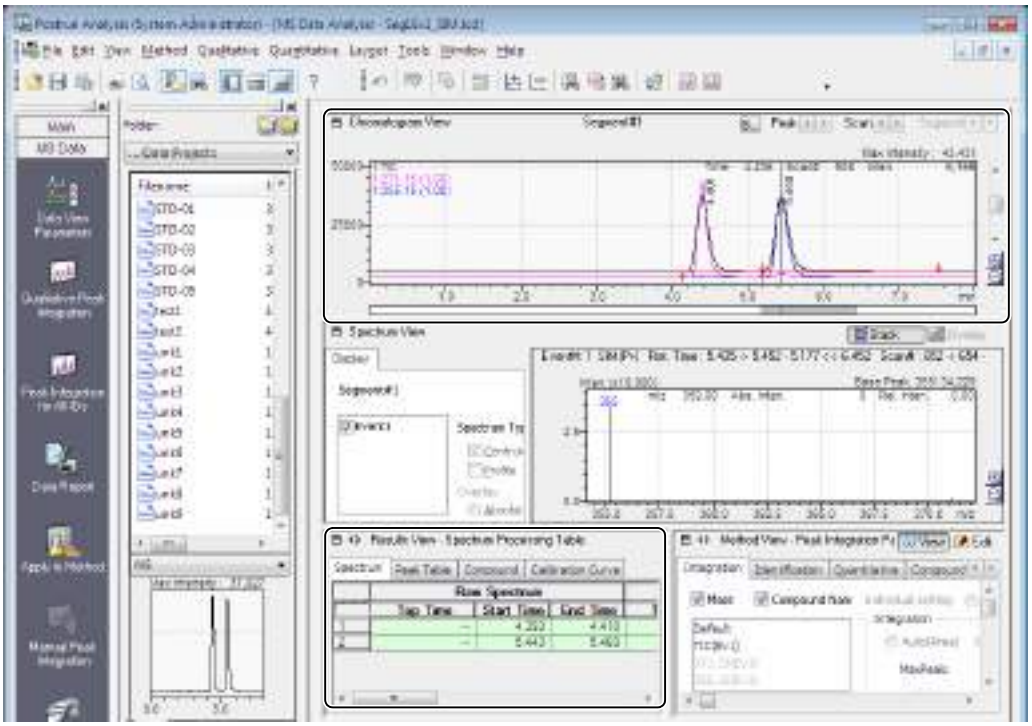



1 If data acquisition was performed with multiple segments, click to change the target segment.

2 Select how detected peaks are registered to the Spectrum Process Table on the [Spectrum] in [Results View].

3 Select [Proc.] to perform peak integration for the chromatogram at the selected *m/z*.

The base line and peak top comment are displayed in [Chromatogram View], and the results of qualitative peak integration are displayed on the [Spectrum] and [Peak Table] tabs in [Results View].



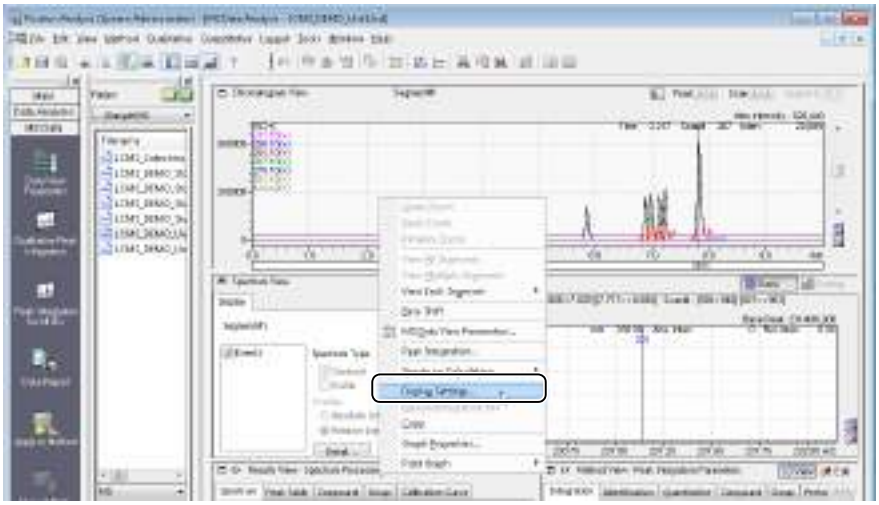
**Reference**

Refer to *"Peak Top Comments" P.186* in *"6.2.4 Change the [Chromatogram View] Display Mode"* if peak top comments are not displayed on the chromatogram.

## 6.3.2 Manual Qualitative Peak Integration

Peak integration can be performed manually if the peaks are not detected with peak integration parameters. This section describes how to manually insert peaks.

**1** **Right-click on [Chromatogram View], and click [Display Settings].**

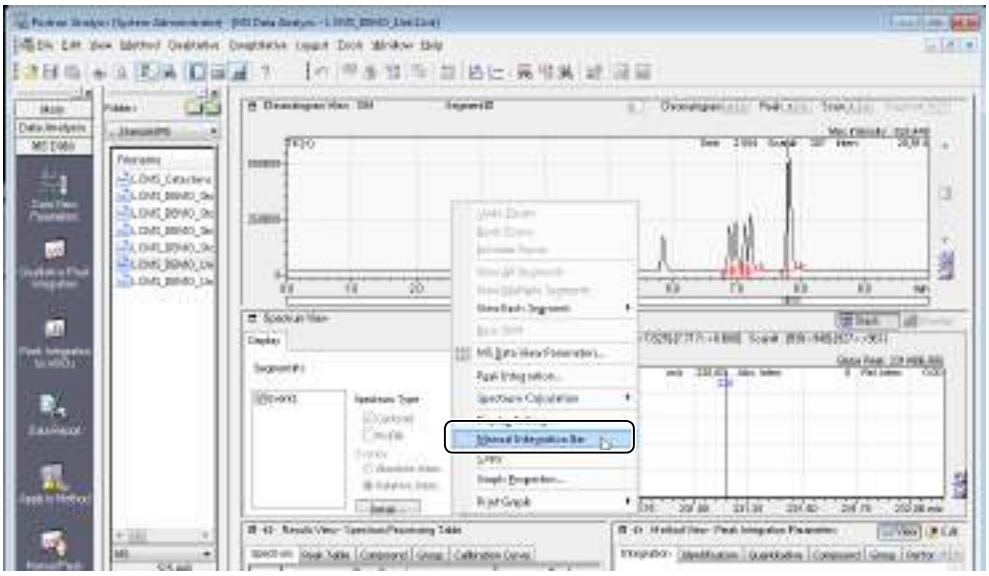


**2** **Set the chromatogram display mode to [Stack] or [Single], and click [OK].**

**NOTE**

The [Manual Integration Bar] cannot be displayed for overlaid chromatograms. Set the display mode to [Stack] or [Single] to perform manual peak integration.

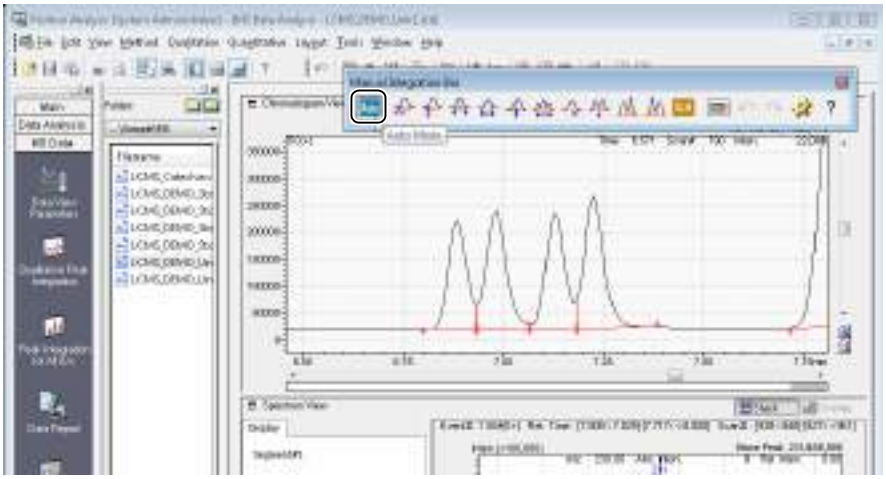
**3** **Right-click on [Chromatogram View], and select [Manual Integration Bar].**



**NOTE**

The [Manual Integration Bar] can also be displayed by selecting [Manual Integration Bar] on the [View] menu in the [MS Data Analysis] window.

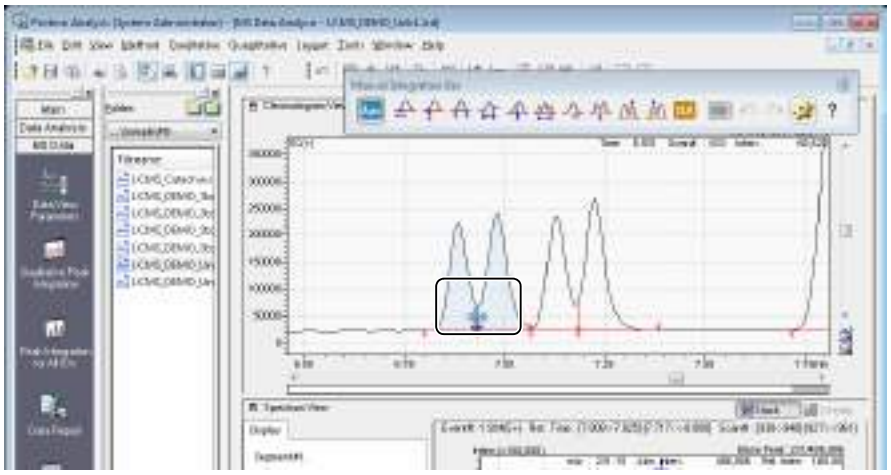
**4** **Click the Auto (Auto Mode) icon.**



**Reference**

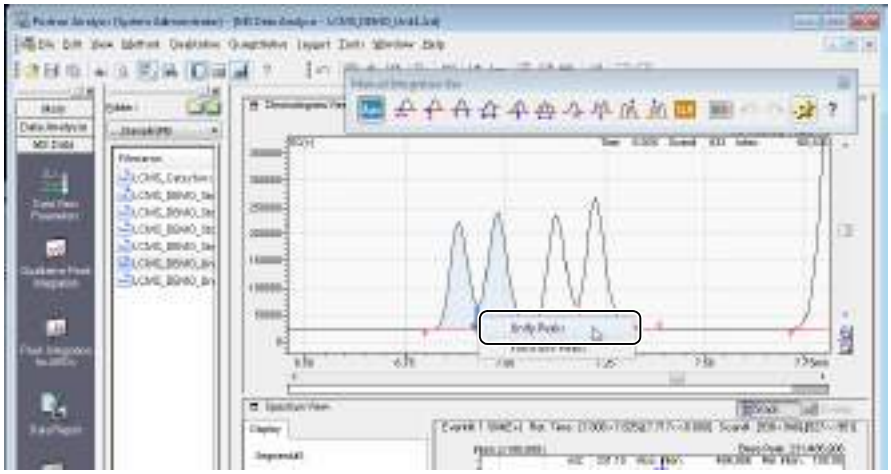
Refer to *"4.2.4 Manual Peak Integration" P.93* for details about the icons.

**5** **Move the mouse to near the vertical division line to unify.**

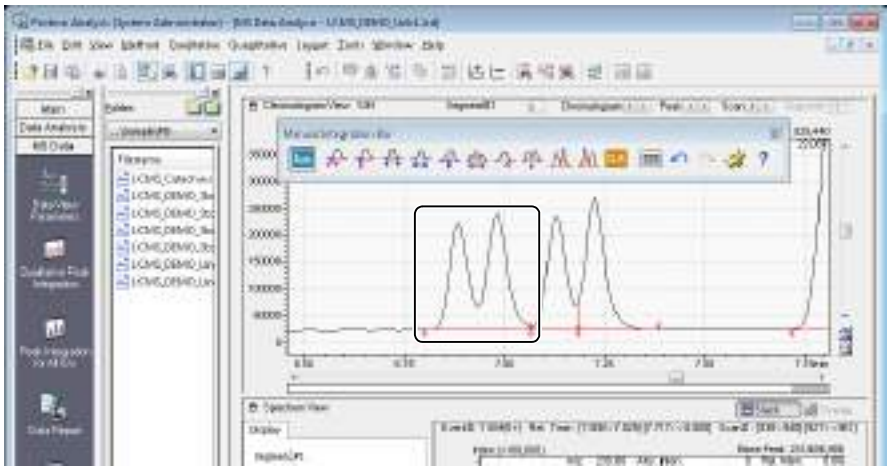


The vertical division line is highlighted.

**6** **Right-click on the graph, and click [Unify Peaks] on the displayed menu.**



The peak is unified.



**NOTE**

- Peaks can be unified using (Unify Peaks) icon.

- The peak integration processing command can also be executed on multiple peaks as a single peak by changing the [Width] value on the [Integration] tab page in [Method View].

**Reference**

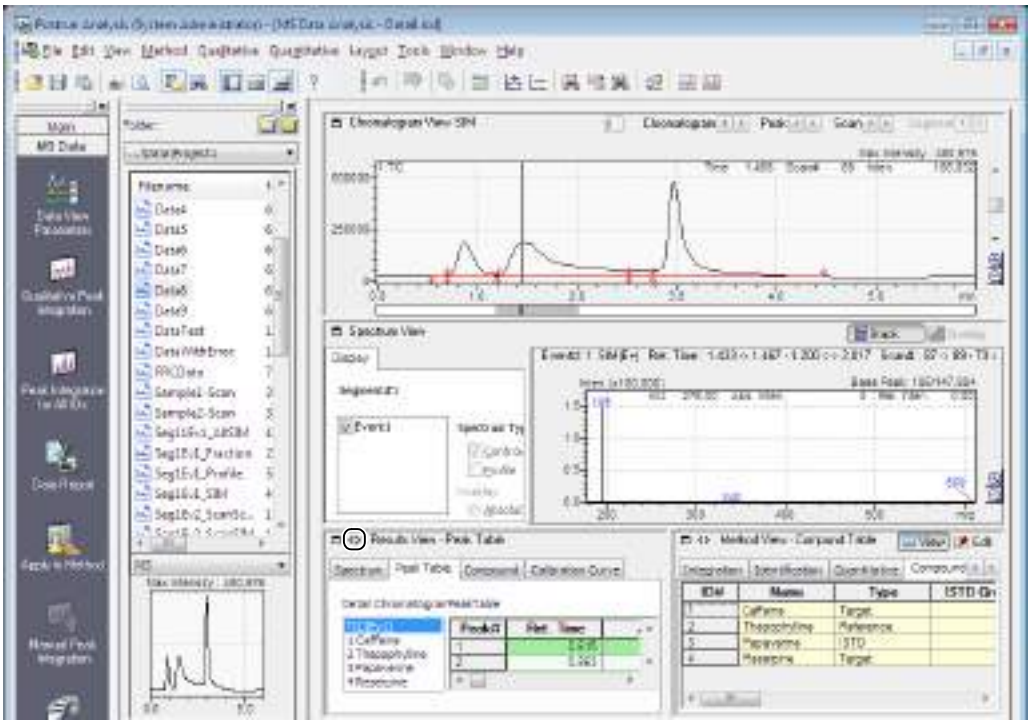
For details on the [Width] value, refer to Help.

**7** **Click to close the [Manual Integration Bar].**

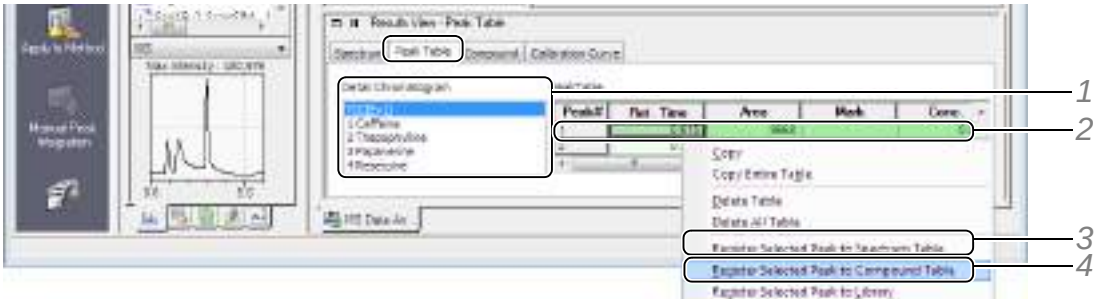
## 6.3.3 Check Peak Integration Results in the Peak Table

Use the Peak Table to display the results of peak integration, and register selected peaks to the Spectrum Process and Compound Tables.

**1** **Click (Wide Size) in [Results View].**



**2** **Click the [Peak Table] tab in [Results View].**




*1* Select the integrated chromatogram.

The peak integration results in the Compound Table are displayed by compound name.

*2* Click a row on the Peak Table, and verify the peak information in [Chromatogram View] or [Spectrum View].

3 Right-click on the row to register to the Spectrum Process Table, and click [Register Selected Peak to Spectrum Table].

The information is registered to the Spectrum Process Table on the [Spectrum] tab in [Results View].

4 Right-click on the row to register to the Compound Table, and click [Register Selected Peak to Compound Table].

The information is registered to the Compound Table on the [Compound] tab in [Method View].

**NOTE**

Right-click on the Peak Table and click [Table Style] to select the items to be displayed in the Peak Table.

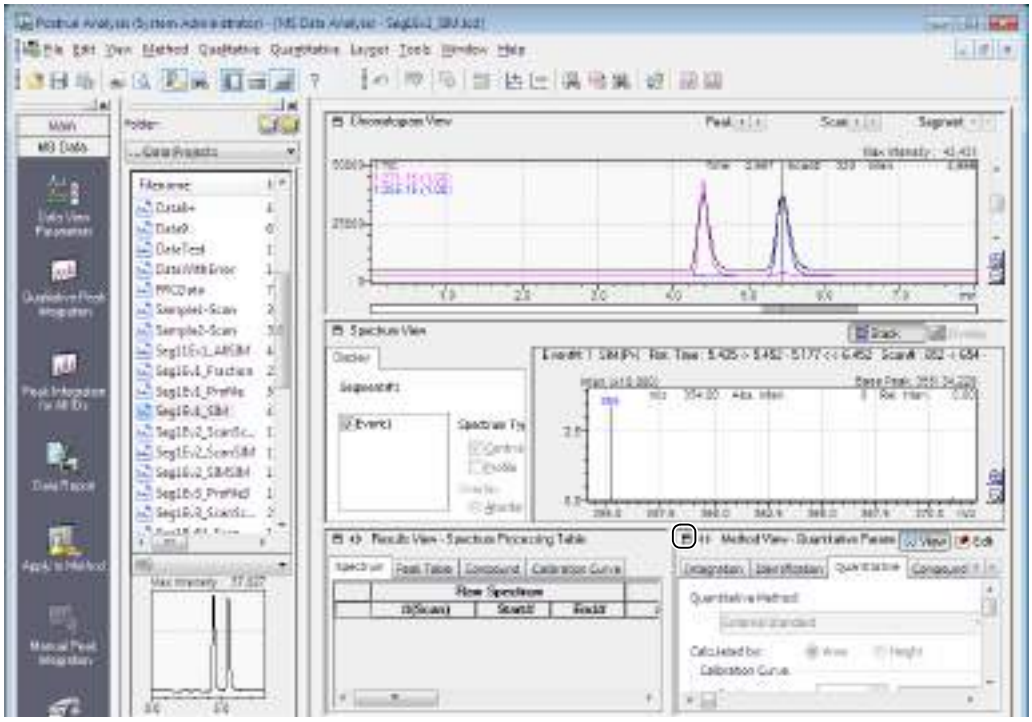
## 6.3.4 MS Spectrum Library Searches

Use library searches to select spectra from MS library files with a high similarity to the spectrum of the detected peak. Use a specific search index as the search key to further filter the library spectra search. Libraries can be searched using [Library] or [(MSn)Library].

This section describes how to perform spectra library searches in [Spectrum View] and in the Spectrum Process Table.

### ■ Library Searches in [Spectrum View]

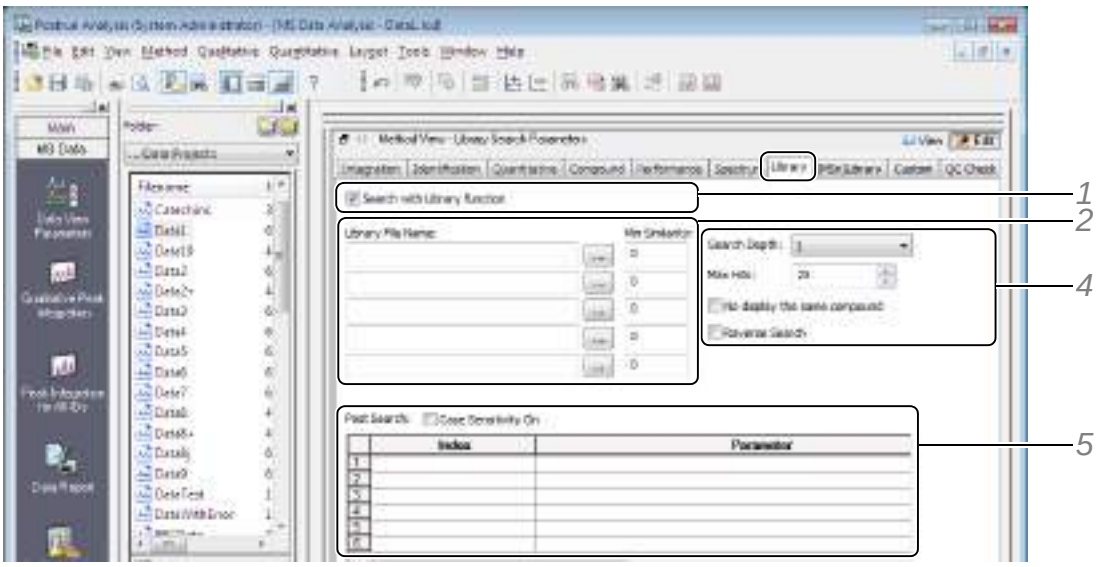
**1** **Click (Full Size) in [Method View].**



**2** **Click Edit (Edit Mode) in [Method View].**

## 3 Click the [Library] tab or the [(MSn)Library] tab, and set each parameter.

### ■ [Library] tab




1 Select [Search with Library function].

2 Click [...] under [Library File Name] to select the files to be searched.
Up to 5 MS library files can be entered. [Min Similarity] can be set for each of the MS library files.

3 Enter [File name], and click [Open].

4 Set the [Search Depth] and [Max Hits]. [Search Depth] specifies the range of important peak groups to target in the search, and [Max Hits] specifies the number of search result that are output.

5 Set the search conditions to perform a filtered library search according to the index information, such as molecular weight and compound name.

■ **[(MSn)Library] tab**

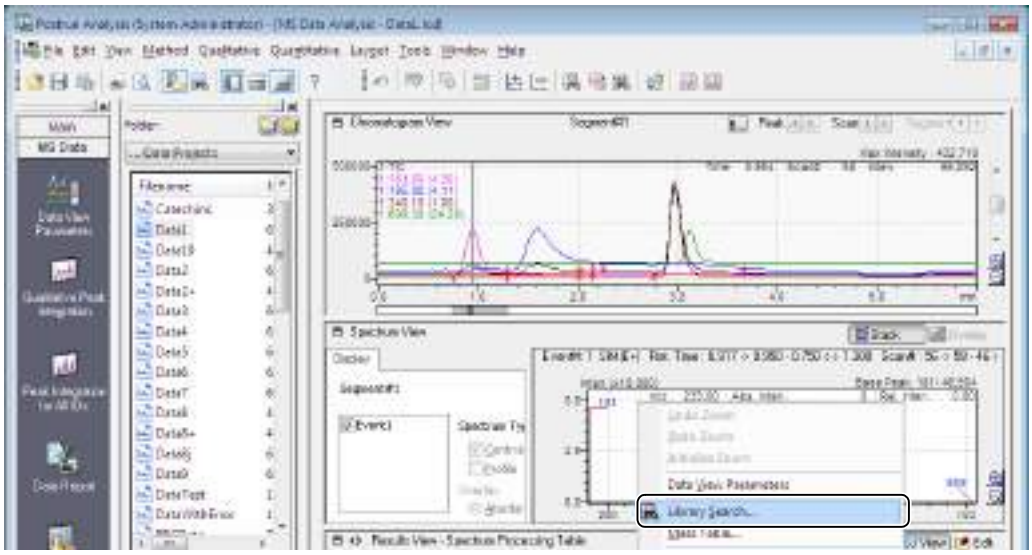
1 Select [Search with (MSn)Library function].

2 Click [...] under [Library File Name] to select the files to be searched.
Up to 5 MSn library files can be entered. [Min Similarity] can be set for each of the MS library files.

3 Enter [File name], and click [Open].

**4 Click [View] (View Mode) in [Method View], and click (Normal Size).**

**5 Right-click on the spectrum in [Spectrum View], and click [Library Search].**



The [Library Search Results] sub-window or [(MSn) Library Search Results] sub-window is displayed.

**Reference**

Refer to *"6.3.5 Check the Library Search Results" P.211* for details on the [Library Search Results] sub-window or [(MSn) Library Search Results] sub-window.

## ■ Library Searches in the Spectrum Process Table

A batch library search can be performed on multiple spectra in the Spectrum Process Table.

**NOTE**

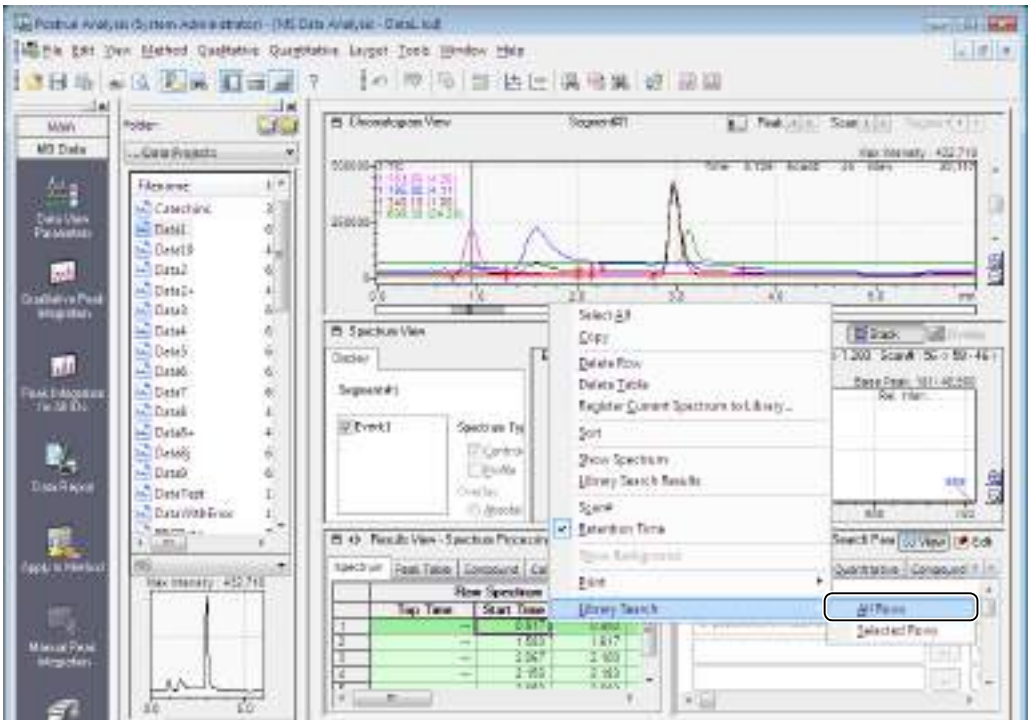
Set the MS library files on the [Library] tab in [Method View]. Refer to *"Library Searches in [Spectrum View]" P.207* in *"6.3.4 MS Spectrum Library Searches"* for details on how to set MS library files.

**1** **Register the spectra to be searched from the library in the Spectrum Process Table.**

**Reference**

Refer to *"6.2.9 Add Spectra to the Spectrum Process Table" P.196* for details on registering spectra to the Spectrum Process Table.

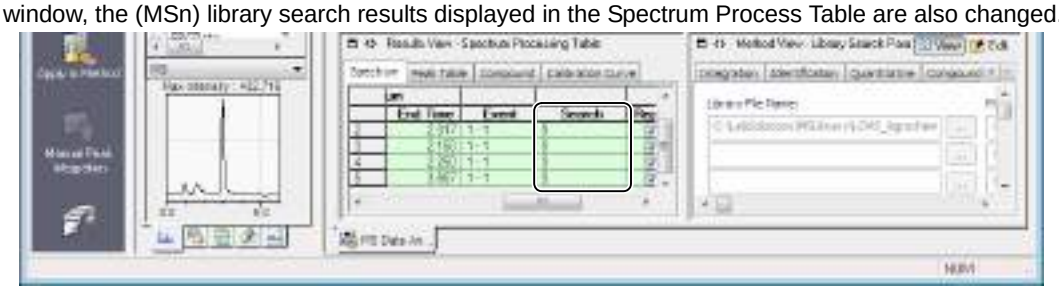
**2** **Right-click on the Spectrum Process Table on the [Spectrum] tab in [Results View], select [Library Search], and click [All Rows].**



**NOTE**

- Right-click the row of the spectrum to perform the library search on, select [Library Search] and click [Selected Rows]. The library search is performed only on the spectrum registered to that row.
- Library searches can also be performed on the spectra of multiple rows. Select all of the rows with the [Shift] or [Ctrl] key held down then right-click and select [Selected Rows] at [Library Search].

The library search is performed for all spectra in the Spectrum Process Table with an “S” or a “M” displayed in the [Search] field. The (MSn) library search results with the largest similarity are displayed in the Spectrum Process Table. When a [Report] field is changed in the [(MSn) Library Search Results] sub-window, the (MSn) library search results displayed in the Spectrum Process Table are also changed.



**3** **Double-click the library-searched row.**

The [Library Search Results] sub-window or [(MSn) Library Search Results] sub-window is displayed.

**NOTE**

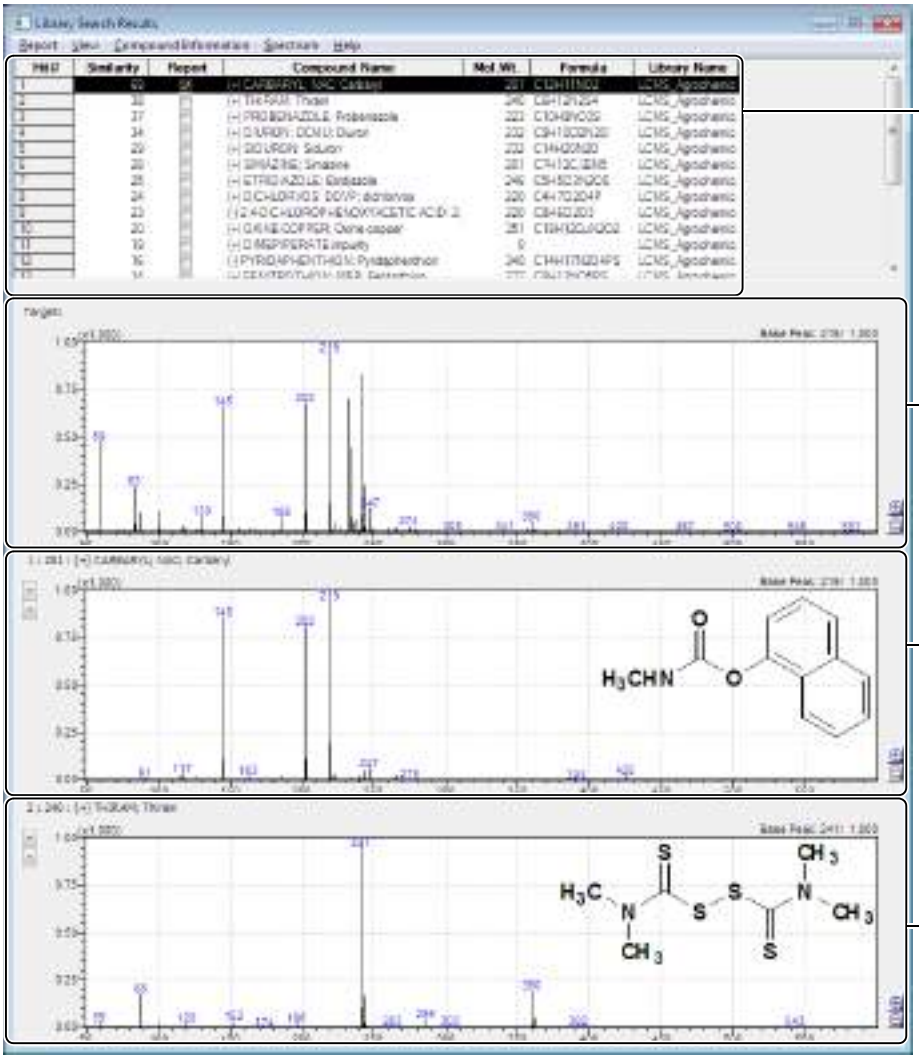
The [Library Search Results] sub-window or [(MSn) Library Search Results] sub-window can also be displayed by right-clicking on a library-searched row, and clicking [Library Search Results].

Performing either library search or (MSn) library search depends on the settings on the [Library] tab or [(MSn)Library] tab in [Method View]. Refer to *"Library Searches in [Spectrum View]" P.207* in the*"6.3.4 MS Spectrum Library Searches"*.

## 6.3.5 Check the Library Search Results

This section describes how to view the [Library Search Results] described in *"6.3.4 MS Spectrum Library Searches" P.207*.

- [Library Search Results] sub-window



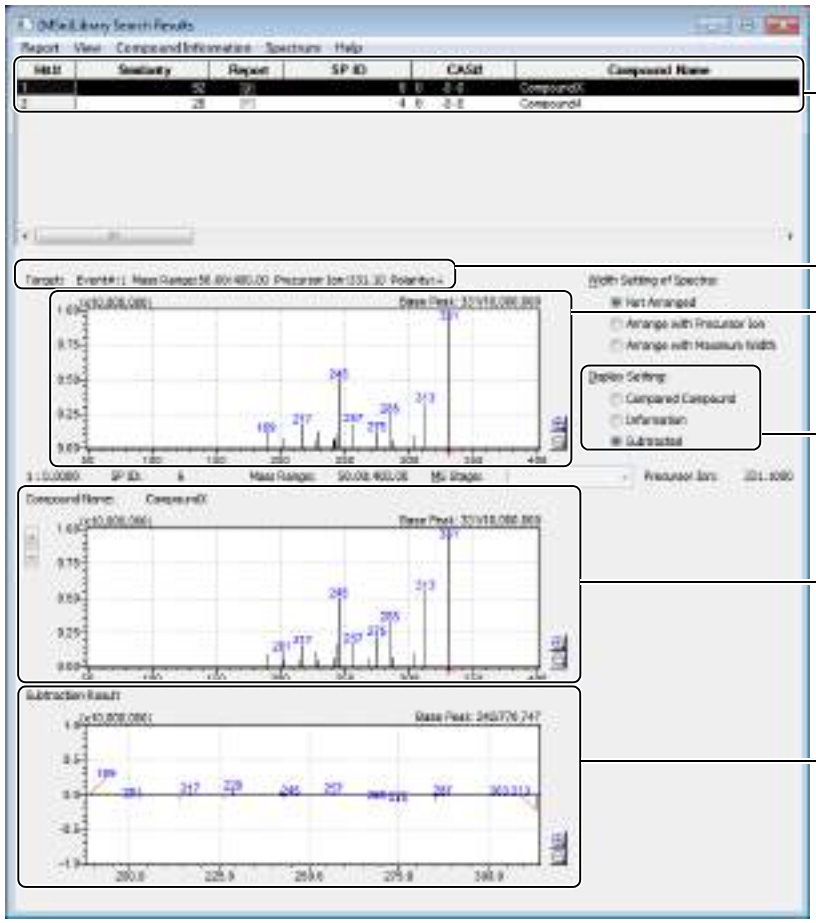

| No. | Explanation |
|---|---|
| 1 | Displays a list of the search results. Compounds are displayed in order from the highest similarity to the lowest. |
| 2 | Displays the target spectrum. |
| 3 | Displays the selected library spectra found in the library search. Click the button on the left of the graph to display the next library spectra in the search result list. |

| No. | Explanation |
|---|---|
| 4 | Displays the compare result spectra, compound information and subtraction result spectra. Click the button on the left of the compare result spectra to display the next library spectra in the search result list. The spectra obtained by subtracting the library spectrum from the target spectrum are displayed. |

**NOTE**

Right-click on the spectrum in the [Library Search Results] sub-window, and click [Compare], [Information] and [Subtract] to change the display content.

- [(MSn)Library Search Results] sub-window




| No. | Explanation |
|---|---|
| 1 | Compounds are displayed in order from the highest similarity to the lowest.<br>The spectrum of the selected row is displayed in the (4) area. |
| 2 | When the library search results of the Spectrum Process Table are displayed, the compound names selected in the [Report] field can be reflected in the compound name cells of the Spectrum Process Table which the data were called from. |
| 3 | Displays the library spectrum of the selected row. Display can be switched by clicking p or q on the left side of the graph. |
| 4 | Sets the contents to display in (6).<br>[Compared Compound]: Displays the spectrum specified in the library.<br>[Information]: Displays the details on the library spectrum currently displayed in (4).<br>[Subtracted]: Displays the differential spectrum for the target spectrum and the library spectrum. |
| 5 | Displays the contents which are set in the [Display Setting] area shown in (5) |

# 6.4 Edit the Private Library

The libraries, which are used for searching mass spectra acquired by the mass spectrometer, are created or maintained in the [MS Library Editor] or [(MSn) MS Library Editor] window. The libraries are saved in different format files depending on MS library search or MSn library search.

## 6.4.1 Display the MS Library Editor Window

### ■ Display the MS Library Editor Window

Click the 

(MS Library Editor) on the [Main] assistant bar to display the [MS Library Editor] sub-window.

### ■ Display the (MSn) MS Library Editor Window

Click the 

((MSn)MS Library Editor) on the [Main] assistant bar to display the [MSn Library Editor] sub-window.

## 6.4.2 Handle the Libraries

This section describes the basic methods to handle the libraries. The methods can be used both in the [MS Library Editor] and [MSn Library Editor] windows.

### ■ Create a New Library

1. **Click the (New) on the toolbar or click [New Library File] on the [File] menu.**
   The [Create New File] sub-window is displayed.

2. **Enter the file name and click [Save].**
   A new library file is created.
   When editing library files directly, refer to "Open the Library" below and open the MS library that was created.

### ■ Open the Library

Click (Open) on the toolbar or click [Open Library File] on the [File] menu.

### ■ Close the Library

Click [Close Library File] on the [File] menu.

**NOTE**

- When the library is changed, the changes are saved in a temporary library. (The menu to save the library does not exist.)
- As the default setting, the (MSn) library files are saved in the [MSLibary] folder where LabSolutions is installed. Since the MS library files are frequently shared, they are not the projects (folders) to be browsed in the [Data Explorer] sub-window but managed in one place.

## 6.4.3 Register a Spectrum in a Library

Register a spectrum to a private library from the [MS Data Analysis] window as follows.

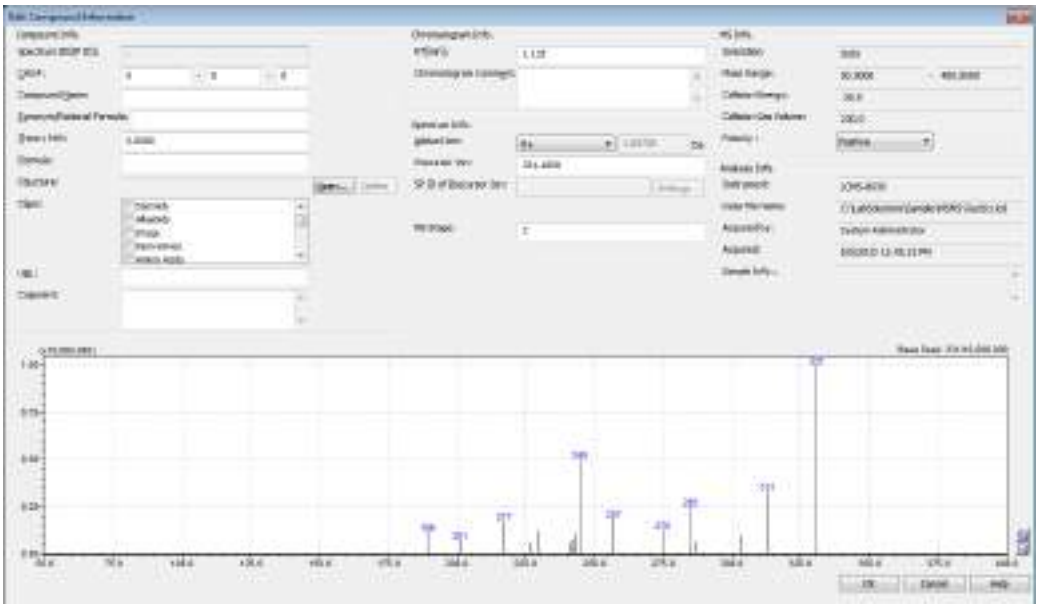
**1** **Display the spectrum to register in [Spectrum View]. Right-click on the [Spectrum View] and click [Register Spectrum to Library] or [(MSn) Register Spectrum to Library] on the displayed menu.**

After the [Select Library] sub-window is displayed, select the library file in which the spectrum will be registered.

**2** **Edit the compound information.**

- When the destination to register a spectrum is MS library

- When the destination to register a spectrum is MSn library



**3** **Set each item and click [OK].**

## 6.4.4 Convert MS library to MSn library

MS Library file (.lib) cannot be used in (MSn) MS library search features.
This section describes how to convert MS Library file to (MSn) MS library file.

1. **Open MS library file (lib) file in the [MS Library Editor] window.**
2. **Click [Convert MLB Library File] on the [File] menu.**
3. **Specify the [File name], and click [Save].**

**NOTE**

- In (MSn) MS library search feature, information that can be registered in the library is increasing, such as precursor ion. Therefore it is recommended that original spectrum should be registered into (MSn) MS library from the original data file.
- In (MSn) MS library search feature, algorithm for calculating the similarity score is different from the MS library search feature. Therefore, both target spectrum and library spectrum is same, similarity may be different from MS library search and (MSn) MS library search.

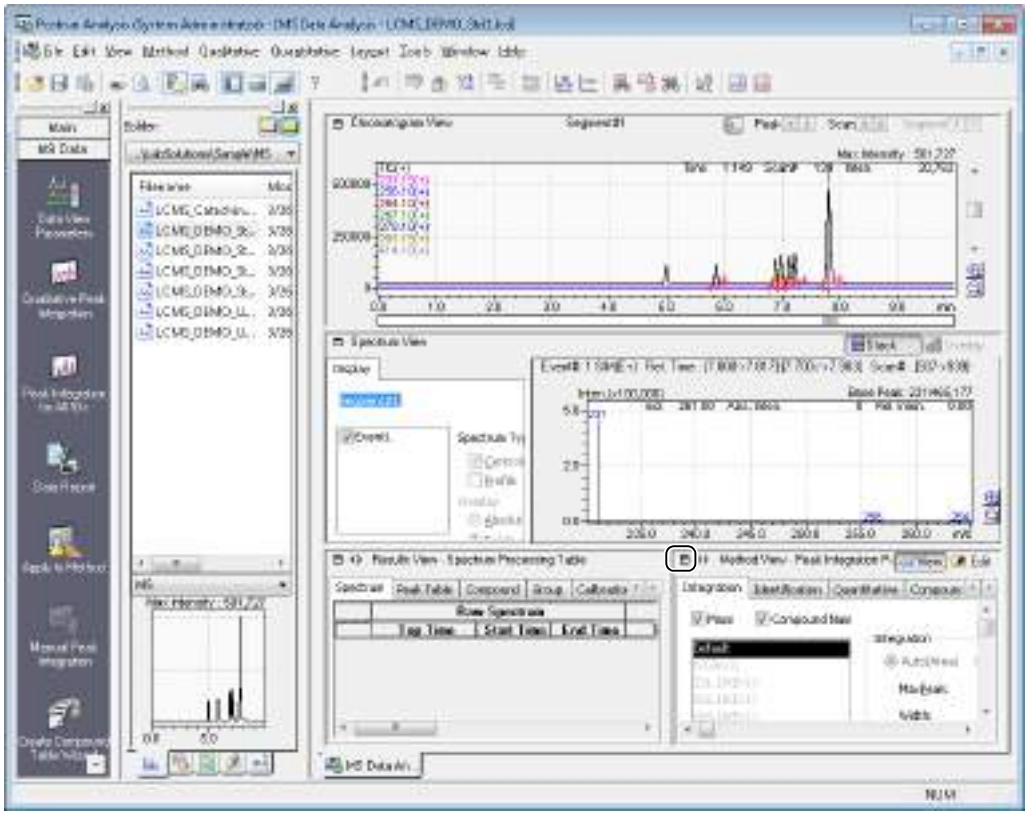
# 6.5 Quantitative Processing

This section describes how to set quantitative parameters to perform quantitative processing. The chromatogram displayed on the [Compound] tab in [Results View] is targeted for processing. The processing results are displayed on the [Compound] and [Calibration Curve] tabs in [Results View].

## 6.5.1 Edit Quantitative Parameters and Compound Tables

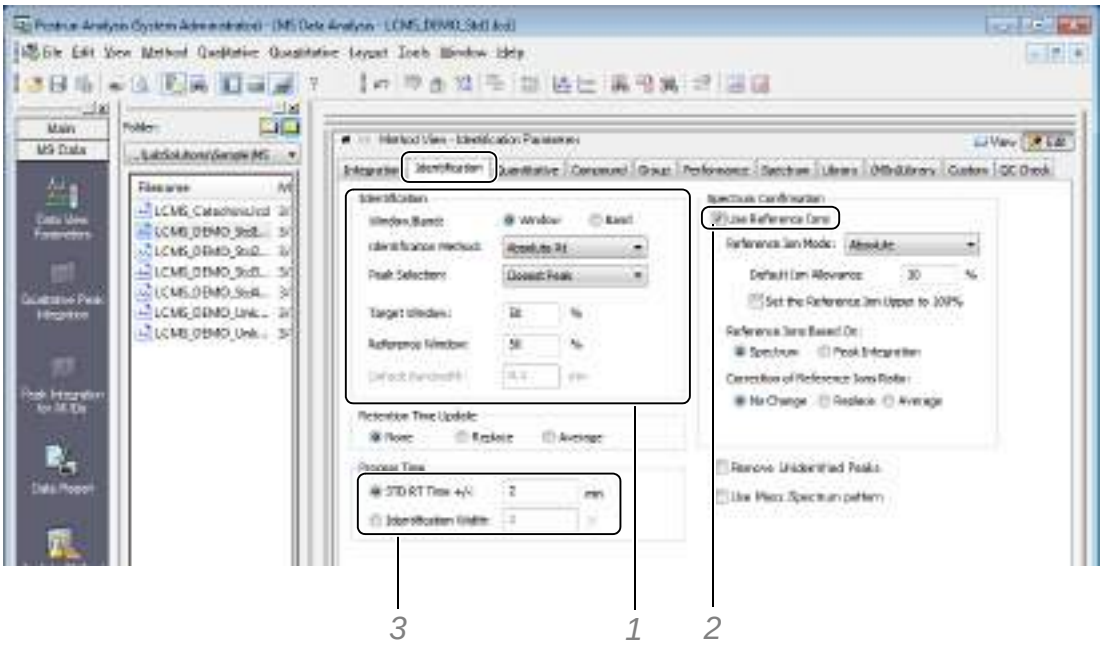
Edit the parameters and Compound Table that are required for quantitative processing. This section describes how to perform quantitation using a 4-point calibration curve by the internal standard method.

**1** **Click (Full Size) in [Method View].**



**2** **Click Edit (Edit Mode) in [Method View].**

## 3 Click the [Identification] tab, and set each parameter.




1 Set the quantitative method and identification tolerance range for the retention time in the Compound Table.

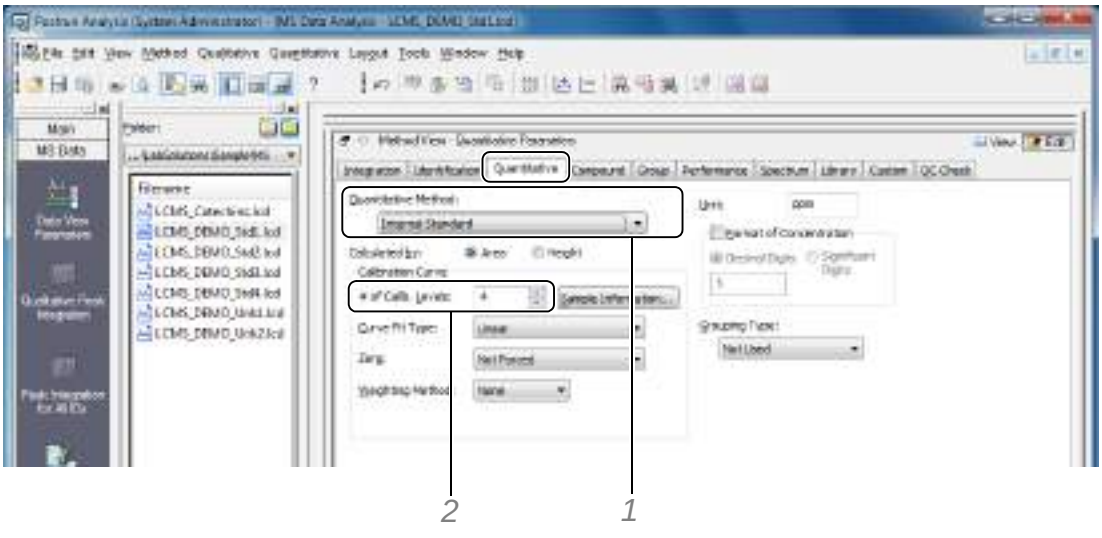
2 Select the [Use Reference Ions] checkbox to perform the spectrum identification.

**Reference**

Refer to *"6.8 Use a Spectrum for Peak Identification" P.236* for details on the spectrum identification.

3 Set the time width of the chromatograms to be displayed on the [Compound] tab page in [Result View].

## 4 Click the [Quantitative] tab, and set each parameter.




1 Select [external Standard] as the [Quantitative Method].

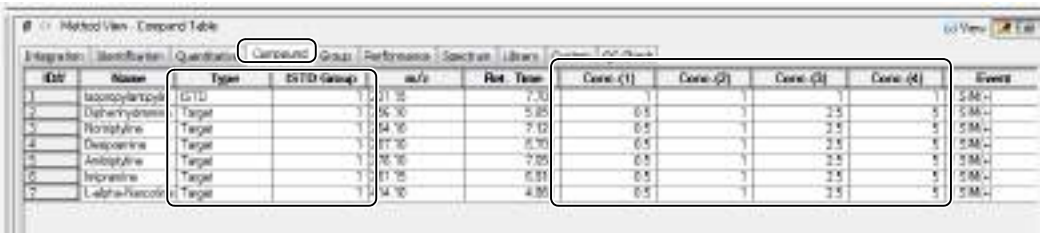
2 Enter the number of concentration levels (number of calibration points) at [# of Calib. Levels].

**NOTE**

If necessary, set the parameters on the [Integration] and [Identification] tabs.

## 5 Click the [Compound] tab, and set [Type], [Conc.], and [ISTD Group] for each compound.

Enter the concentration of the standard sample.



**NOTE**

- Right-click on a Compound Table on the [Compound] tab and click [Table Style] to select the items to be displayed in the Compound Table.
- The ISTD concentration values are used to calculate the calibration curve as the ISTD amount.
- If multiple ISTDs are used, number the substances in the [ISTD Group] column so that the ISTDs corresponding to the target substance are in the same ISTD group.

## 6 Click View (View Mode) in [Method View], and click (Normal Size).

The new parameters are applied.

## 6.5.2 Quantitative Processing on Chromatograms

This section describes how to perform quantitative processing on chromatograms by creating a calibration curve and calculating the concentration values of the target peak.

**NOTE**

Refer to *"6.5.1 Edit Quantitative Parameters and Compound Tables" P.217* to perform quantitative processing and edit the quantitative parameters and Compound Table.

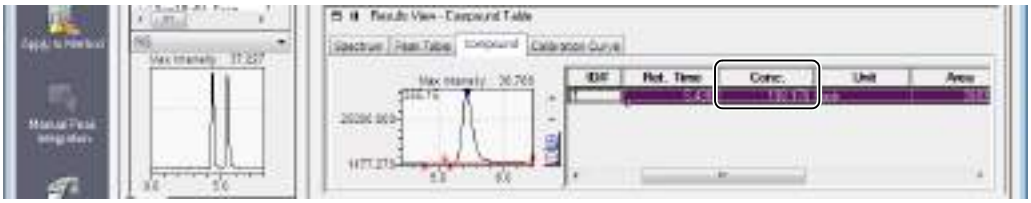
**1** **Click the (Peak Integration for All IDs) icon on the [MS Data] assistant bar.**

The chromatograms undergo quantitative processing (peak integration, identification and quantitative processing) for all of the IDs in the Compound Table on the [Compound] tab in [Method View].

**NOTE**

- Quantitative processing can also be performed by clicking (Peak Integration for All IDs) on the toolbar or by right-clicking on the Compound Result Table and clicking [Peak Integration for All IDs].
- Right-click on the Compound Result Table, and click [Peak Integration for ID #] to perform peak integration for selected IDs in the Compound Result Table.

The results of quantitative calculation are displayed in the [Conc.] field of the Compound Result Table.



**NOTE**

- The [Conc.] displays are the result of multiplying concentrations obtained from the calibration curve by the [Dilution Factor] and dividing the result by the [Sample Amount]. The [Dilution Factor] and [Sample Amount] can be edited on the [Sample Info.] tab in the [Property] sub-window. The [Property] sub-window is displayed by clicking [Data File Properties] on the [File] menu in the [MS Data Analysis] window.
- Click a row in the Compound Result Table to display the information for that compound in [Chromatogram View] and [Spectrum View].
- Right-click on a Compound Table on the [Compound] tab and click [Table Style] to select the items to be displayed in the Compound Table.

## 6.5.3 Calibration Curves

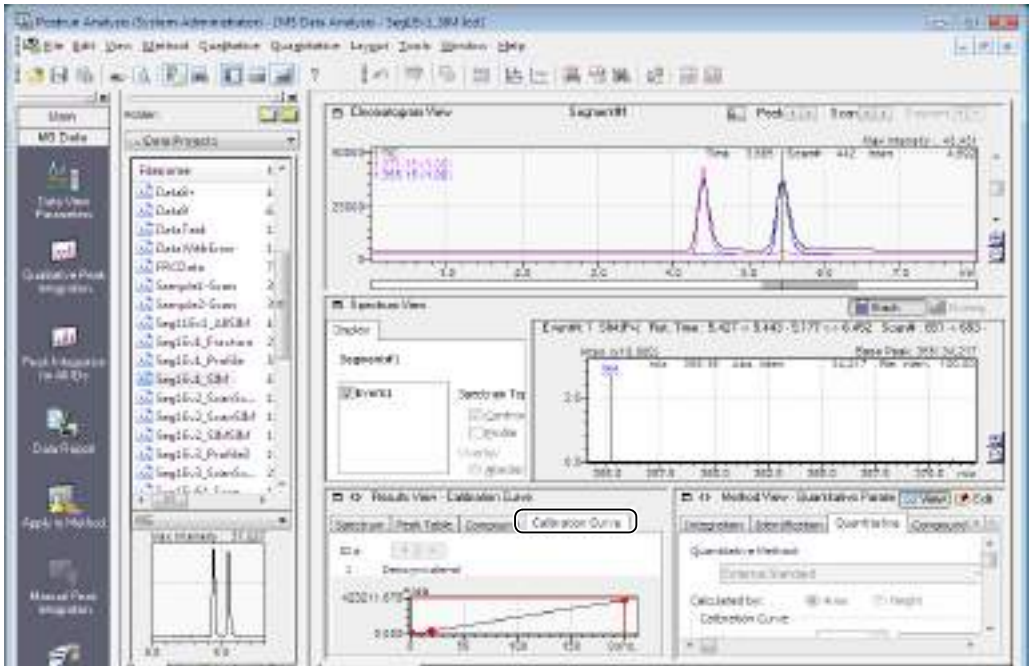
The calibration curves are part of the method information in data files and can be displayed on the [Calibration Curve] tab in [Results View].

**Reference**

Refer to the Data Acquisition & Processing Theory Guide for details on method information in data files.

### ■ Display Calibration Curves

**1** **Click the [Calibration Curve] tab in [Results View].**

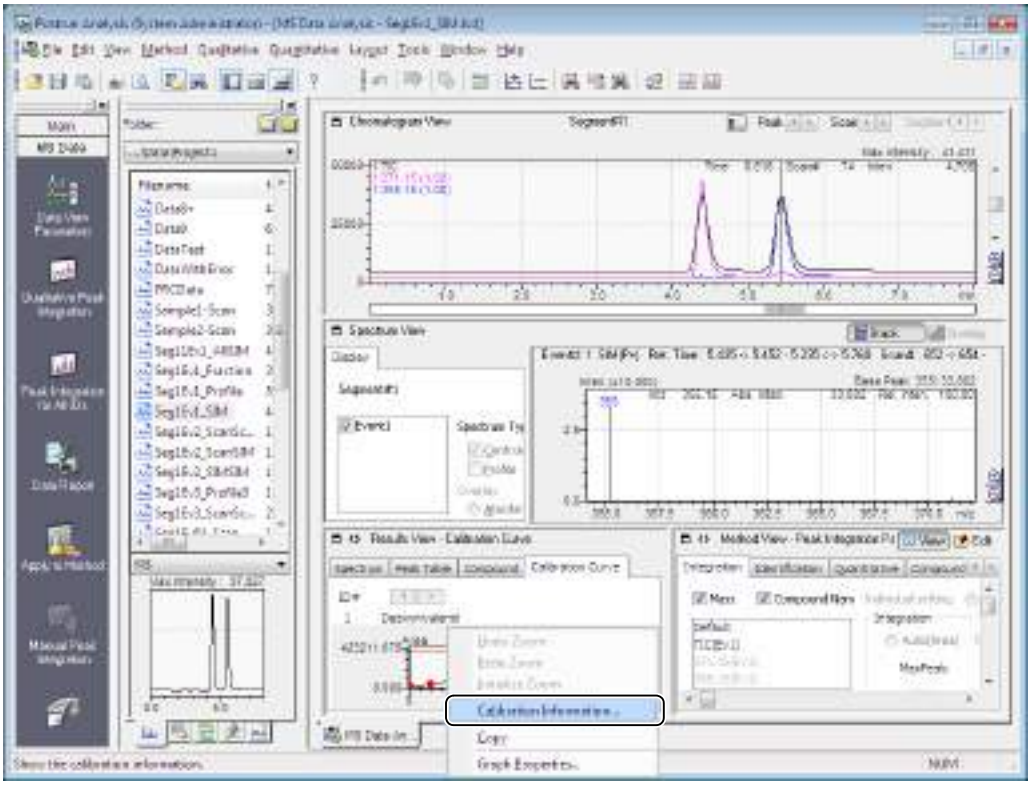


The compound names of the current calibration curve are displayed. Click ◀ ▶ to change the ID and calibration curve.

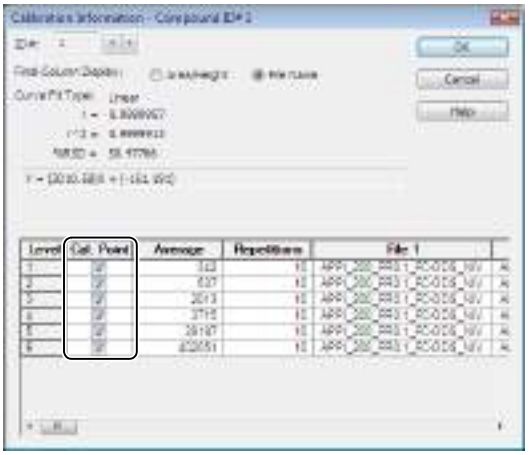
## ■ Disable Calibration Curves

Calibration curves can be disabled if standard samples were not been analyzed appropriately. This section describes how to disable calibration curves.

**1** **Right-click on the calibration curve display area, and click [Calibration Information].**



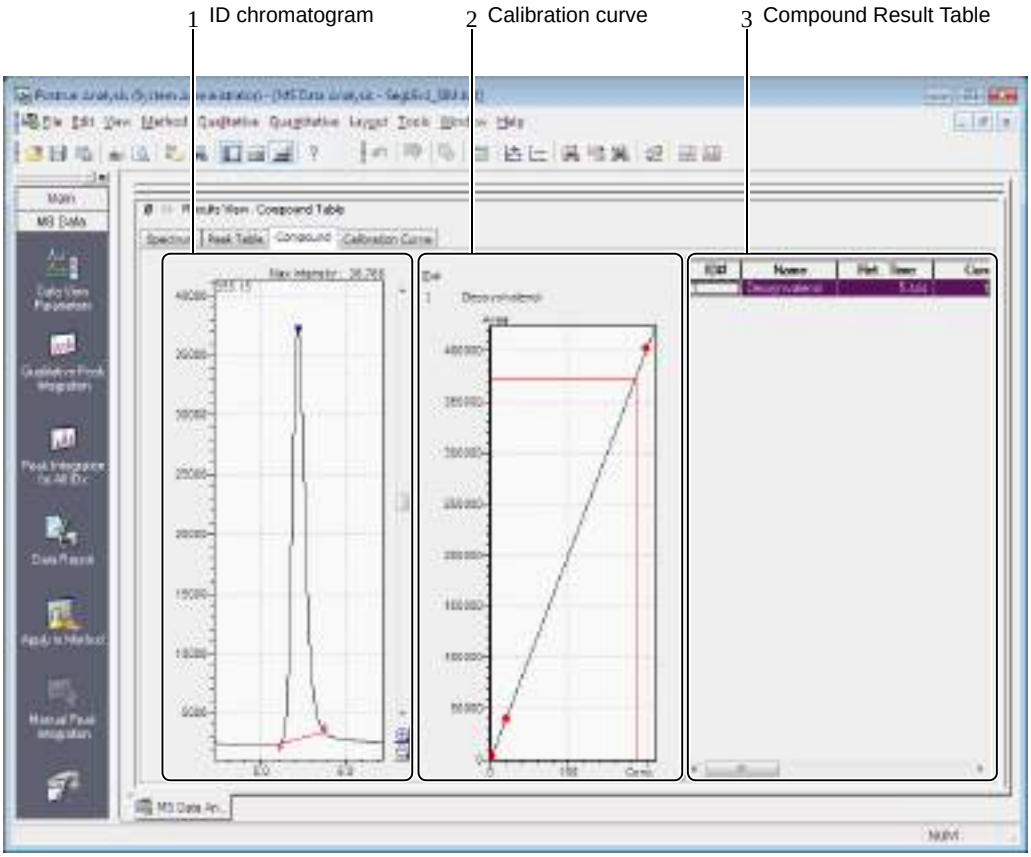
**2** **Deselect [Cal. Point].**



Calibration points whose [Cal. Point] is deselected are disabled, the calibration curve is created again and the concentration re-calculated.

## 6.5.4 Check Quantitative Results on the [Compound] Tab

The quantitative processing results are displayed on the [Compound] tab in [Results View]. The ID chromatogram, calibration curve and Compound Result Table are displayed on the [Compound] tab.




| No. | Explanation |
|---|---|
| 1 | Displays the chromatogram of the compound selected in the Compound Result Table and the spectra of identified peaks are displayed in [Spectrum View]. Double-click the time position to be extracted and the spectrum for that time position is displayed in [Spectrum View]. |
| 2 | Displays the calibration curve of the compound selected in the Compound Result Table. |
| 3 | Displays the result of quantitative processing. |

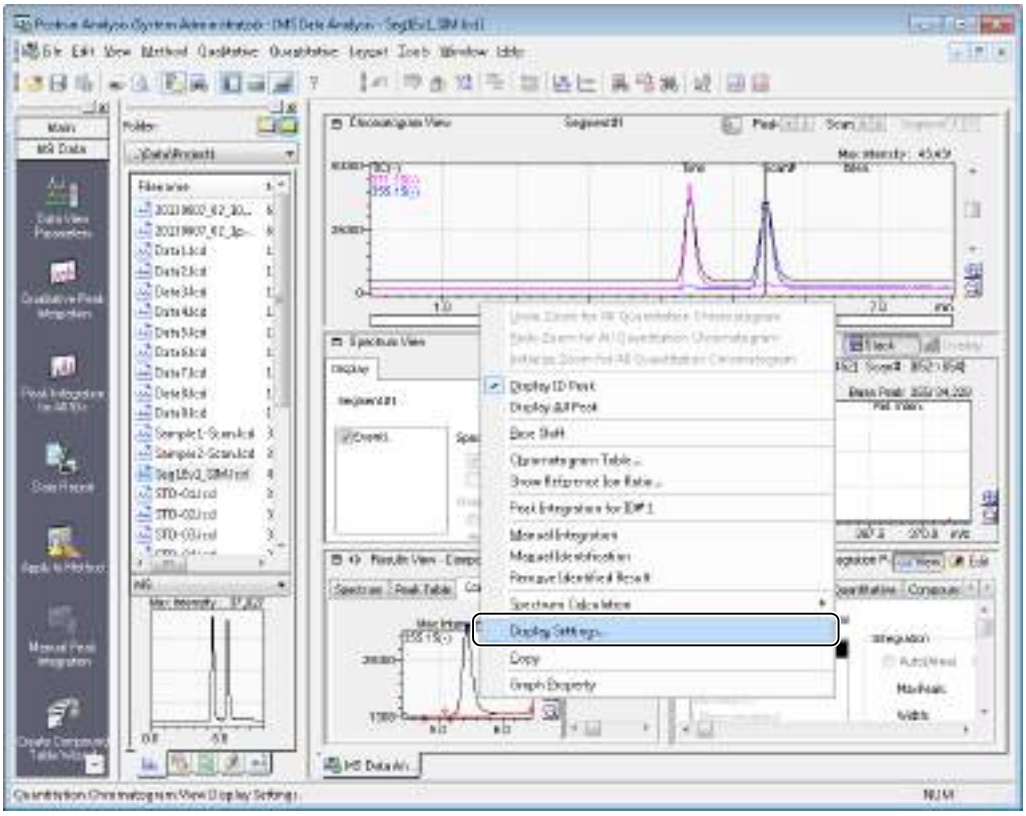
**NOTE**

- The ID chromatogram, calibration curve and Compound Result Table are separated by a divider. Drag these dividers with the mouse to adjust the size of the display areas.
- Calibration curves are not displayed as default. Refer to *"6.5.5 Change the [Compound] Tab Display" P.224* to display calibration curves.

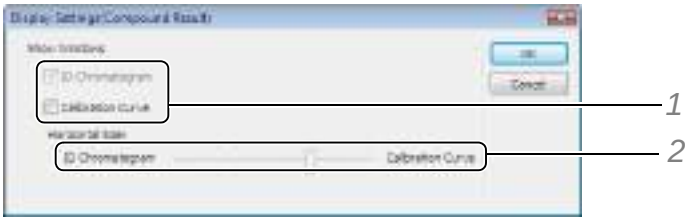
## 6.5.5 Change the [Compound] Tab Display

The ratio between the [ID Chromatogram] and [Calibration Curve] display areas can be changed in the [Display Settings (Compound Results)] sub-window.

**1** **Right-click on Compound Result Table, and click [Display Settings].**




**2** **Set each item, and click [OK].**



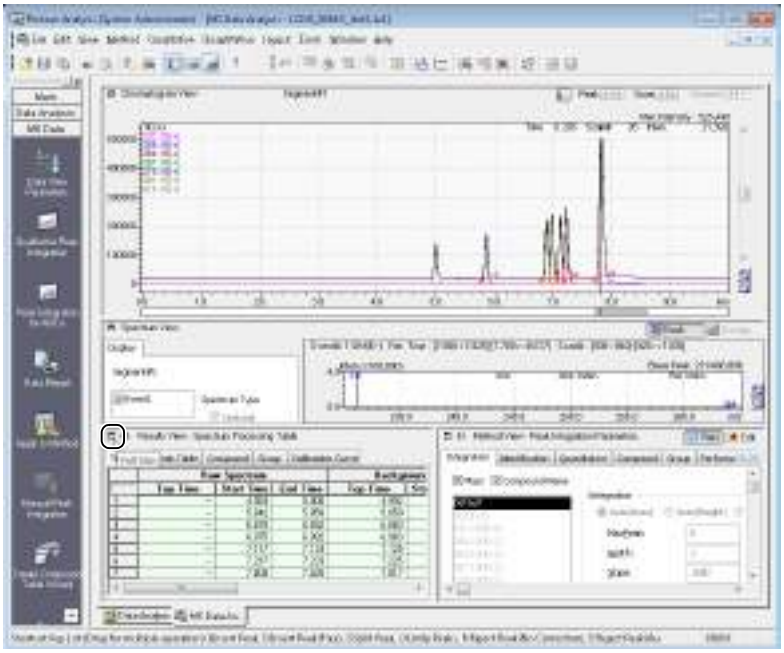

1 Select the checkbox to display [ID Chromatogram] or [Calibration Curve].
2 Set the display ratio in the horizontal direction for both the [ID Chromatogram] and [Calibration Curve].

The [ID Chromatogram] or [Calibration Curve] display is changed.

## 6.5.6 Manual Quantitative Peak Integration

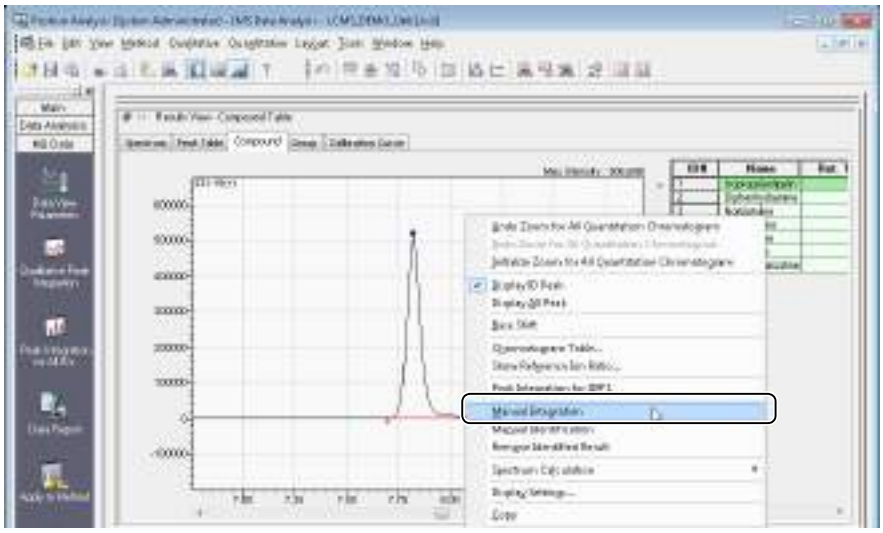
Peak integration can be manually performed if peaks are not be detected with the peak integration parameters. This section describes how to clear the results of peak integration, and manually insert peaks.

**1** **Click (Full Size) in [Results View].**

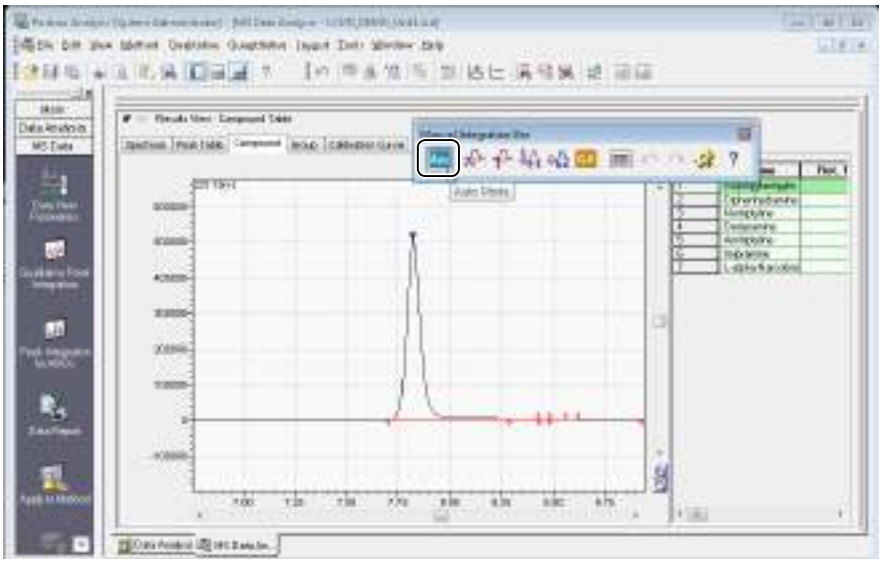


**2** **Refer to *"6.5.5 Change the [Compound] Tab Display"* to change the display to make ID chromatograms, calibration curves and the Compound Result Table easier to view.**

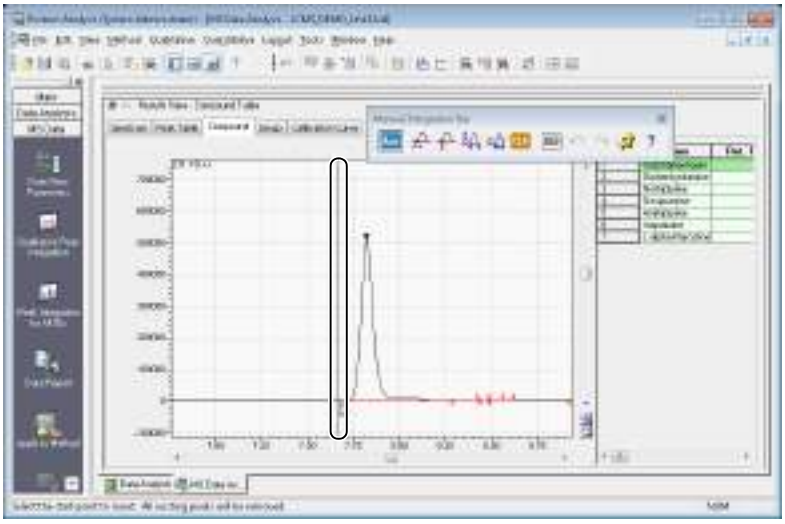
**3** **Right-click on the ID chromatogram on the [Compound] tab, and click [Manual Integration].**



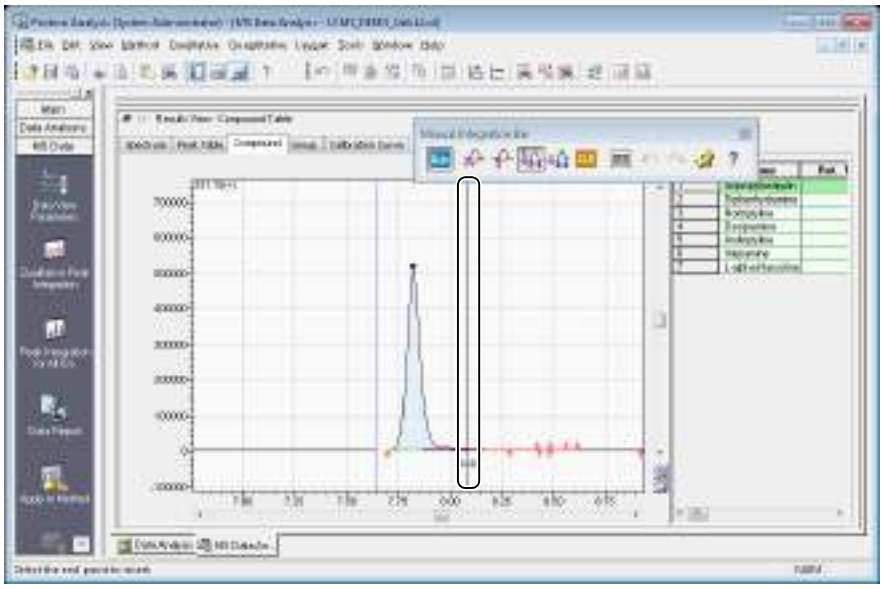
**4** **Click the (Auto Mode) icon.**



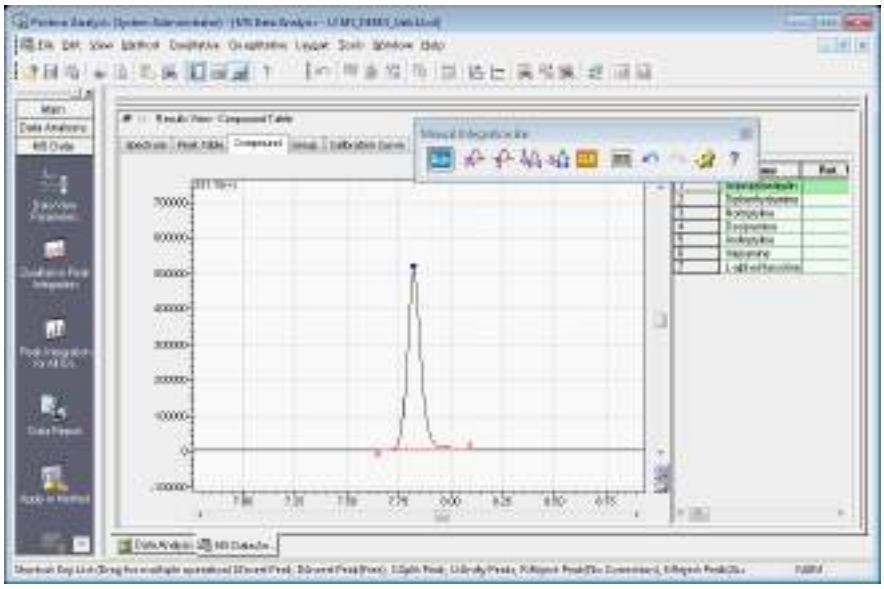
**5** **Move the mouse to the peak start point to insert .**



**6** **Move the mouse to near the peak end point to insert .**



The manual peak integration results are displayed.



**7** **Click to close the [Manual Integration Bar].**

**8** **Click (Normal Size) in [Results View].**

**NOTE**

Peaks can be inserted by using (Clear & Insert Peak) icon.

## 6.5.7 Manual Peak Identification

This section describes how to perform manual identification if the target peak is not successfully identified.

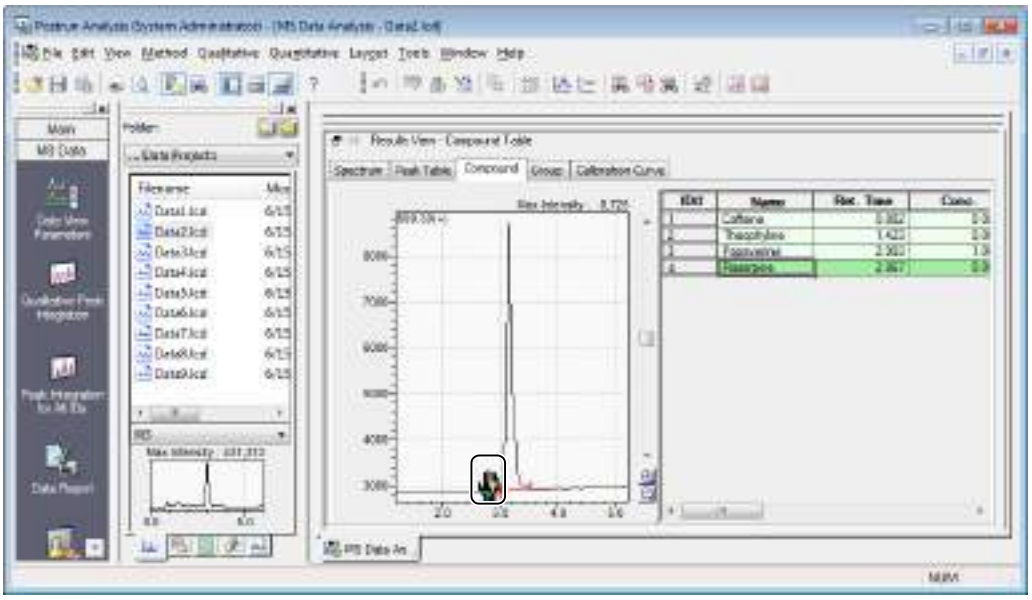
### ■ Correct Identified Peaks

The target peak can be manually changed if another adjacent peak was mistakenly identified.

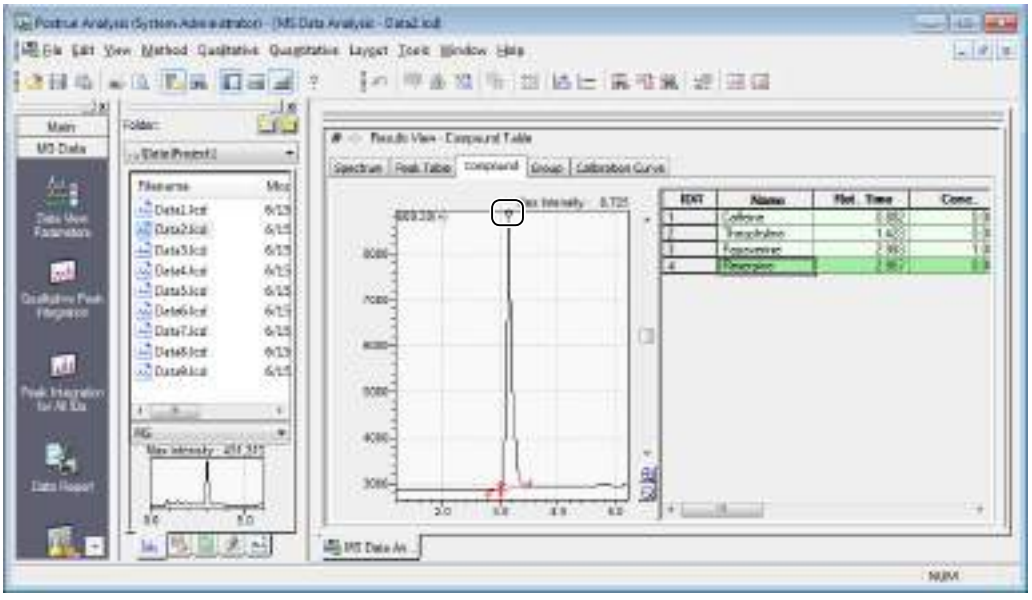
**1** **Use the mouse to drag the ▼ mark at the top of the closest incorrectly identified peak to the top of the peak.**

**NOTE**

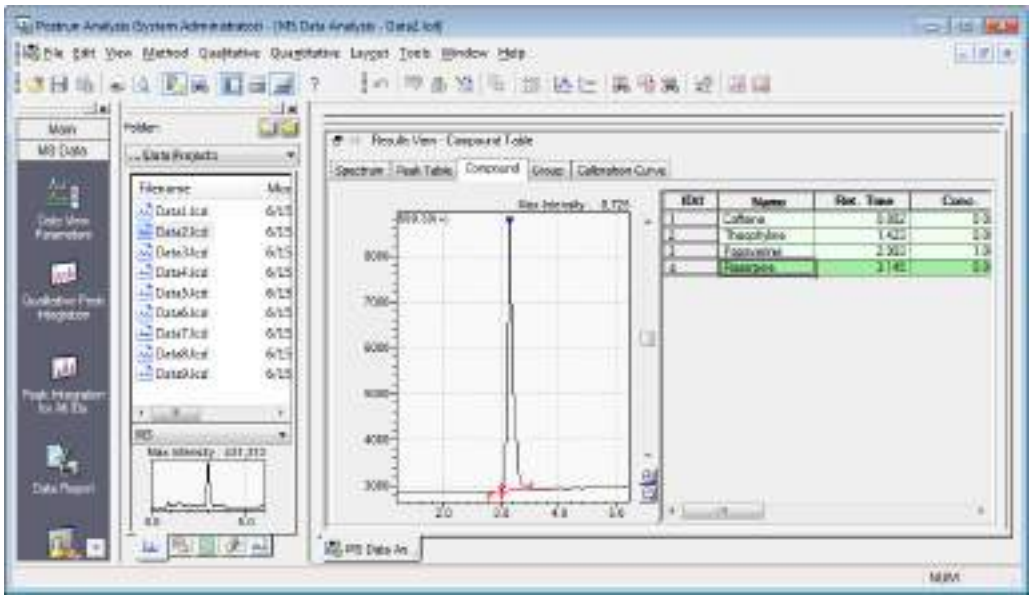
The tops of already identified peaks are marked by the ▼ mark.



**2** **Drop near the top of a new peak.**



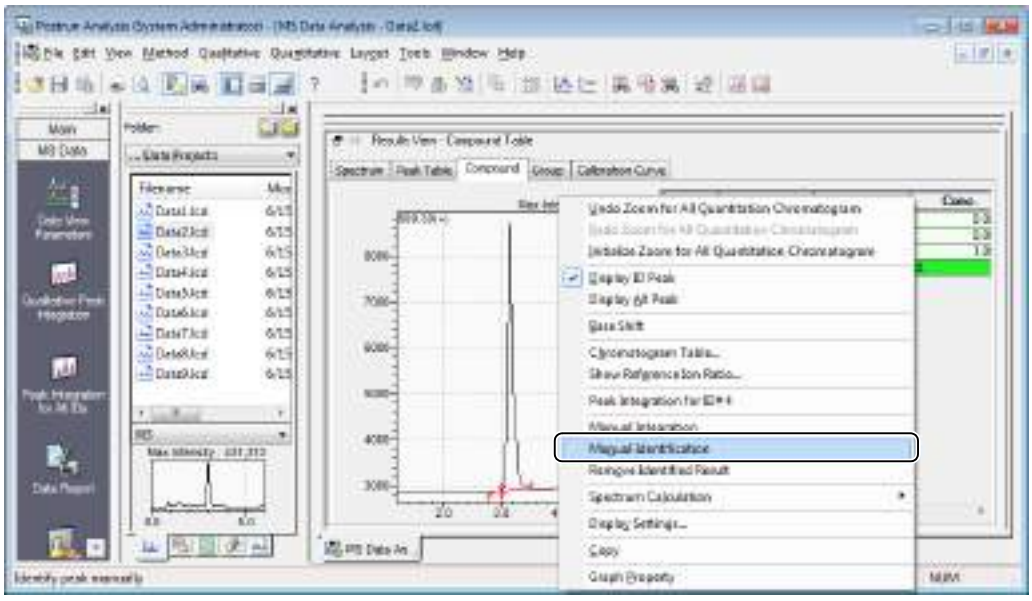
The identified peak is changed and the quantitative results are re-calculated.



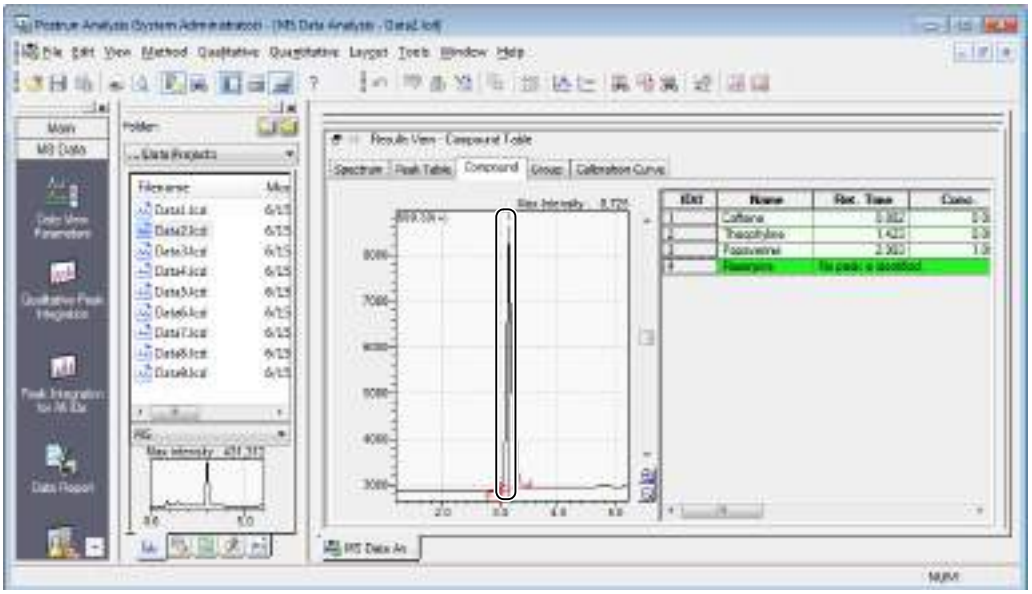
## ■ Manual Identification

Perform manual identification if the peak was detected but not identified.

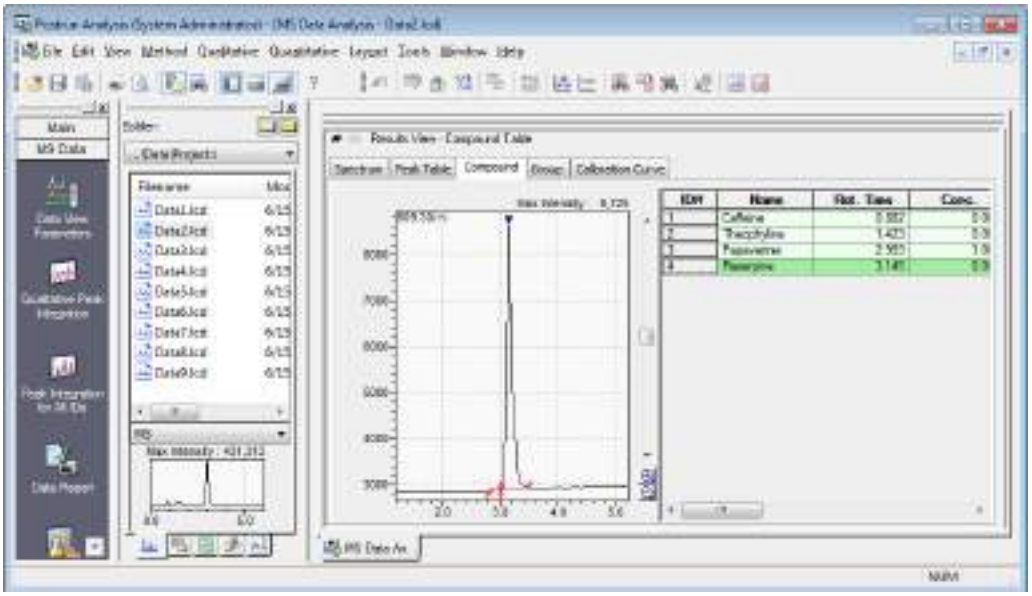
**1** **Right-click on the ID chromatogram on the [Compound] tab, and click [Manual Identification].**



**2** **The cursor changes to a vertical line. Click near the retention time of the peak to identify.**



The peak is identified and the quantitative results are re-calculated and displayed in the Compound Result Table.



**NOTE**

Right-click on the ID chromatogram, and click [Remove Identified Result] to delete identification results.

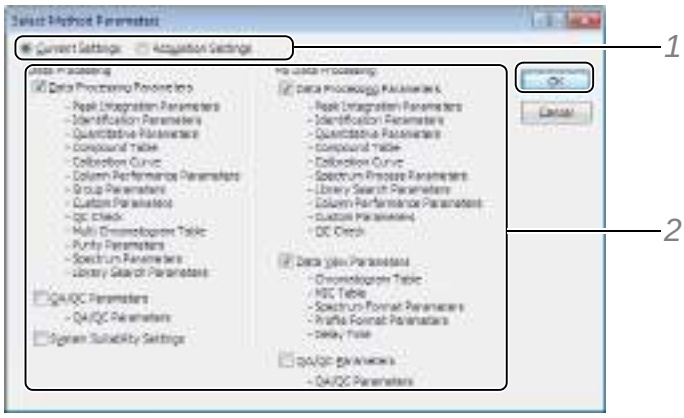
# 6.6 Save Method Files

Changes to the data processing parameters in [Method View] can be saved (exported) to a method file.

**1** **Click the (Apply to Method) icon on the [MS Data] assistant bar.**

**2** **Specify the [File name], and click [Save].**

**3** **Set the [Selected Method Parameters] sub-window, and click [OK].**




*1* [Current Settings] saves the latest method parameters. [Acquisition Settings] saves the method parameters that were used at the time of data acquisition. Select [Current Settings] for this example.

*2* Select the method parameters to save.
The selected method parameters are saved to the method file.

**NOTE**

To open a method file, click [Load Method Parameters] on the [File] menu in the [MS Data Analysis] window, and specify the method file.

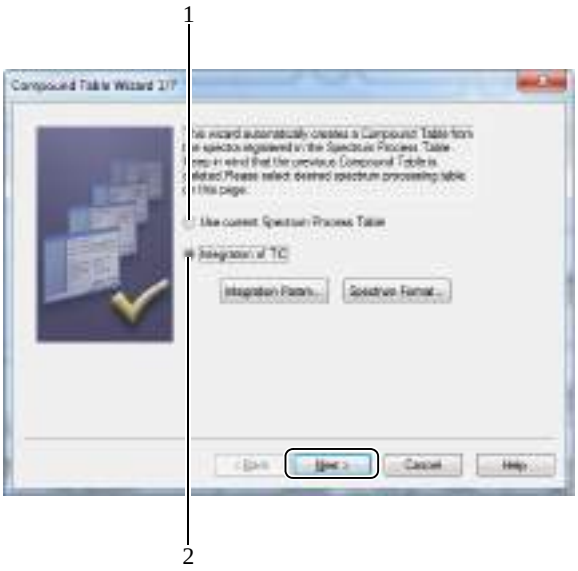
# 6.7 Use the "Compound Table Wizard"

By using the "Compound Table Wizard", [Identification Parameters], [Quantitative Parameters], and [Compound Table] in [Method View] can be set at once. The "Compound Table Wizard" acquires identification conditions, such as peak retention time and spectrums, from the actual data.

**1** **Click the (Create Compound Table Wizard) icon in the [MS Data] assistant bar.**

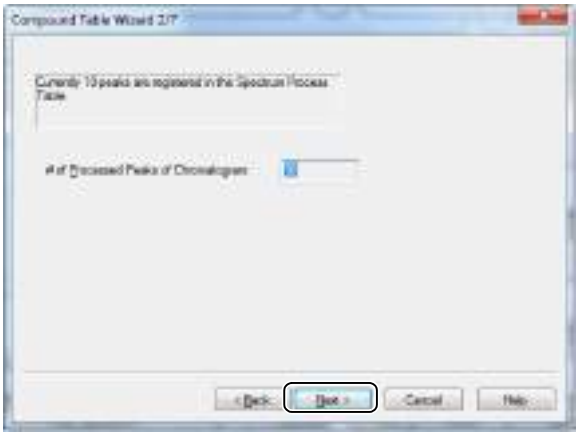
The "Compound Table Wizard" is started.This wizard can be used when [Method View] is in the display mode.

**2** **Select either 1 or 2, and click [Next].**

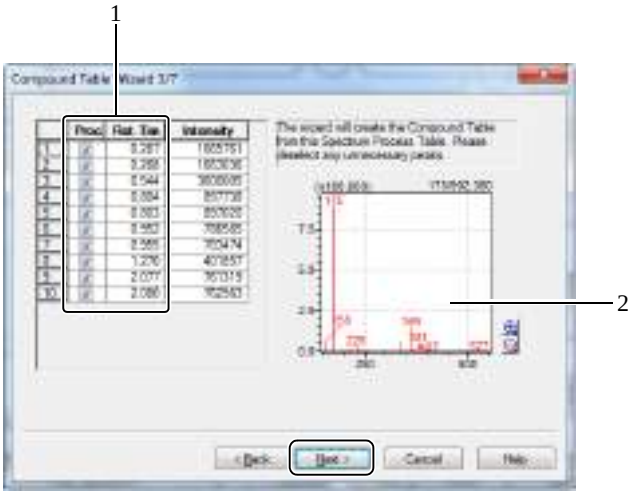



| No. | Description |
|---|---|
| 1 | Creates a compound table using spectrums already registered in the spectrum process table. Before starting the "Compound Table Wizard", register necessary peak spectrums in the spectrum process table. |
| 2 | Creates a compound table using peak spectrums detected by peak integration of the TIC. |

## 3 Check the number of spectrums registered in [Spectrum Process Table], and click [Next].

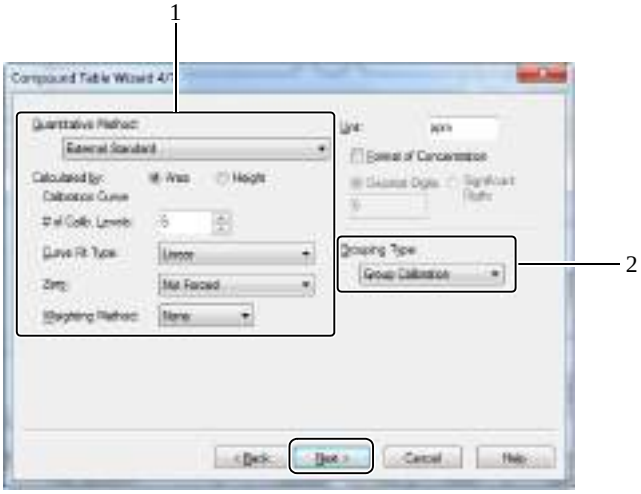


## 4 Select spectrums to process and click [Next].




| No. | Description |
|---|---|
| 1 | Check the retention time of spectrums to use to create a compound table.<br>The peaks around the retention times registered here are calculated. |
| 2 | Displays spectrums according to the rows selected in the table of 1.<br>It works in conjunction with the display of [Chromatogram View] of [MS Data Analysis]. Check the peak cutout, etc. |

## 5 Set each item and click [Next].

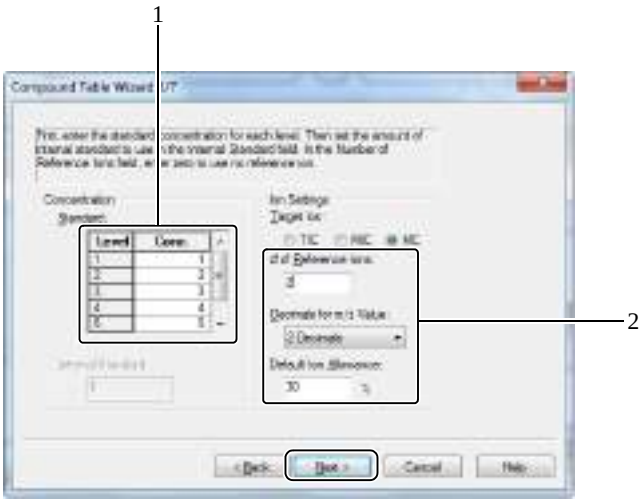



| No. | Description |
|---|---|
| 1 | Specify a quantitative calculation method and a curve type.<br>Set required items.<br>For [Calculated by], select either peak area value or peak height value as the data used for quantitative calculations.<br>For [# of Calib. Levels] at [Calibration Curve], enter the expected number of levels of the calibration curve. |
| 2 | Setting [Group Type] will allow you to quantitatively analyze the following groups in addition to the individual quantitative calculations for each peak:<br>• [Group Calibration]<br>A calibration curve is created from the total area/height of peaks specified in the same group, and used for quantitative analysis.<br>• [Conc. Summation]<br>The sum of concentrations that have been individually obtained by quantitative calculation for the peaks specified in the same group is output. |

### Reference

When grouping type is selected, make settings for each group on the [Group] tab of [Method View] after completing setting in the "Compound Table Wizard".

## 6 Set each item and click [Next].



| No. | Description |
|---|---|
| 1 | In concentration (1), (2), ..., enter level 1 concentration, level 2 concentration, ... of the compound contained in the standard sample.(The "Level" number of each sample to be analyzed must be set to each sample in the Batch Table.) |
| 2 | Specify the peak identification method. |

## 7 Set each item and click [Next].

Complete the detailed settings for each row of [Compound Table].
Enter a component name and a type for the peak to be identified, and register the reference ion.

**NOTE**

When the external standard method is used for quantitative analysis, always specify [Target] for [Type]. For the internal standard method, specify [ISTD] only for the type of the internal standard substance, and enter the same number for the internal standard peak and [ISTD Group] of peaks that are calculated using the internal standard peak in the compound table.

## 8 When the confirmation screen appears, click [Finish].

The "Compound Table Wizard" is completed, and the edited content is reflected in [Compound Table].

## 9 Click View (View Mode) in [Method View].

The edited content is fixed.

**NOTE**

To cancel the edited data, select [Cancel Edit] on the [Edit] menu in the [MS Data Analysis] window before clicking View (View Mode).

# 6.8 Use a Spectrum for Peak Identification

This section explains how to specify the spectrum identification setting in the compound table.

To perform the spectrum identification, set up "reference ion ratio".

## ■ Reference ion ratio identification

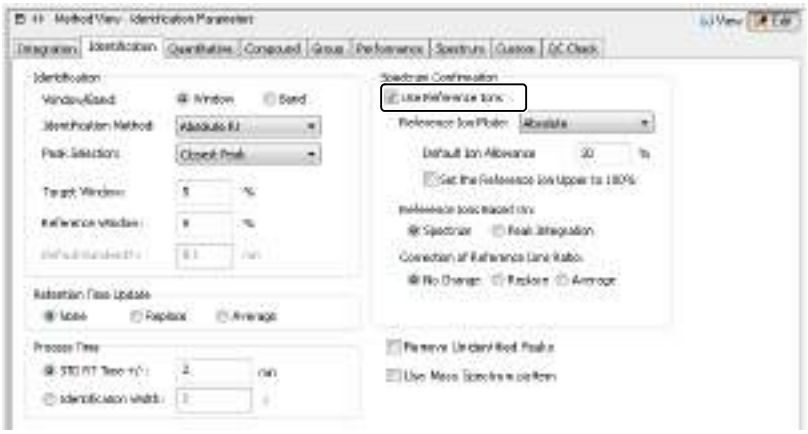
For the ion in [m/z] in [Compound Table] (target ion), the mass of the reference ion and the height ratio/ height acceptable width for the target ion are specified and used for identification.

The reference ion ratio identification may be used with the retention time identification.

### Set the reference ion ratio

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Identification] tab, and select [Use Reference Ions].**



The reference ion identification is enabled.

**3** **Right-click on the [Compound] tab, and select [Set Reference Ion Ratio] from the displayed menu.**

The [Reference Ion Ratio] screen appears.

**4** **Set [m/z], [Ratio], and [Allowance], and click .**

**5** **Click View (View Mode) in [Method View].**

**NOTE**

Clicking [Spectrum View] when the focus bar is displayed in the [m/z] cell sets that *m/z* value.

### Set compound information

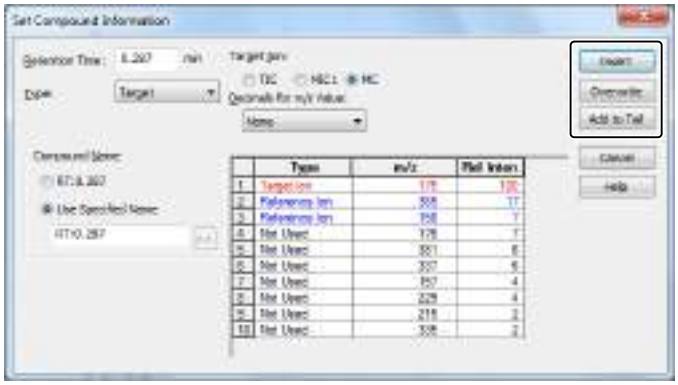
[Set Compound Information] allows you to edit the compound information on one row at once.

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Right-click on the [Compound] tab, and select [Set Compound Information] from the displayed menu.**

The [Set Compound Information] screen appears.

**3** **Set each item, and click one of [Insert], [Overwrite], or [Add to Tail].**

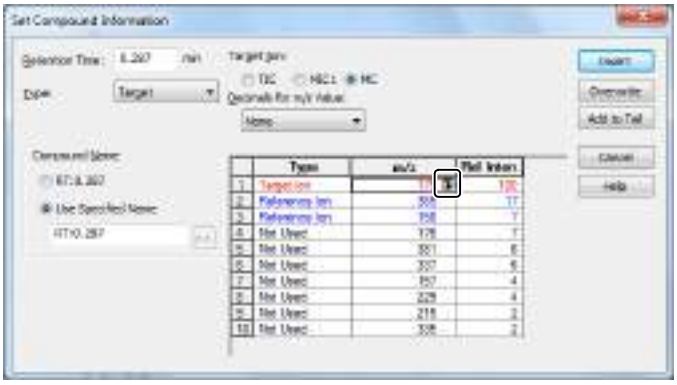


**NOTE**

The list of [Type], [m/z], and [Rel. Inten.] located in the lower right area can be set from the spectrum as follows.

This section describes the procedure to obtain [m/z] as an example.

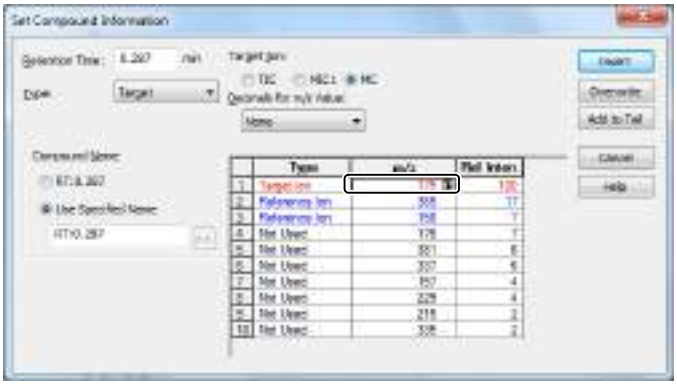
1 Click the [m/z] cell.



The [Pick m/z Value] screen appears.

2 Double-click the spectrum peak of the desired mass position.

The mass is set to the [m/z] cell.



**4 Click View (View Mode) in [Method View].**

# 6.9 Print Data Acquisition Results

The [MS Data Analysis] window has a graph image function to print the [Chromatogram View] and [Spectrum View], and a data report function to print a report according to a specified report format.

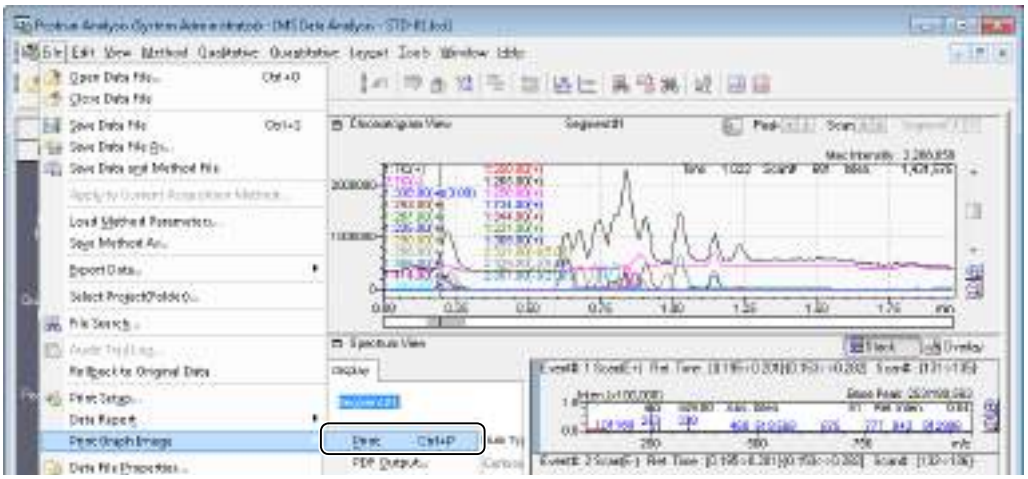
## 6.9.1 Print a Graph Image

This function prints the chromatograms and spectra displayed in the [MS Data Analysis] window.

### ■ Print from the [File] Menu

Select [Print Graph Image] on the [File] menu to print the displayed chromatograms and spectra on a single page.

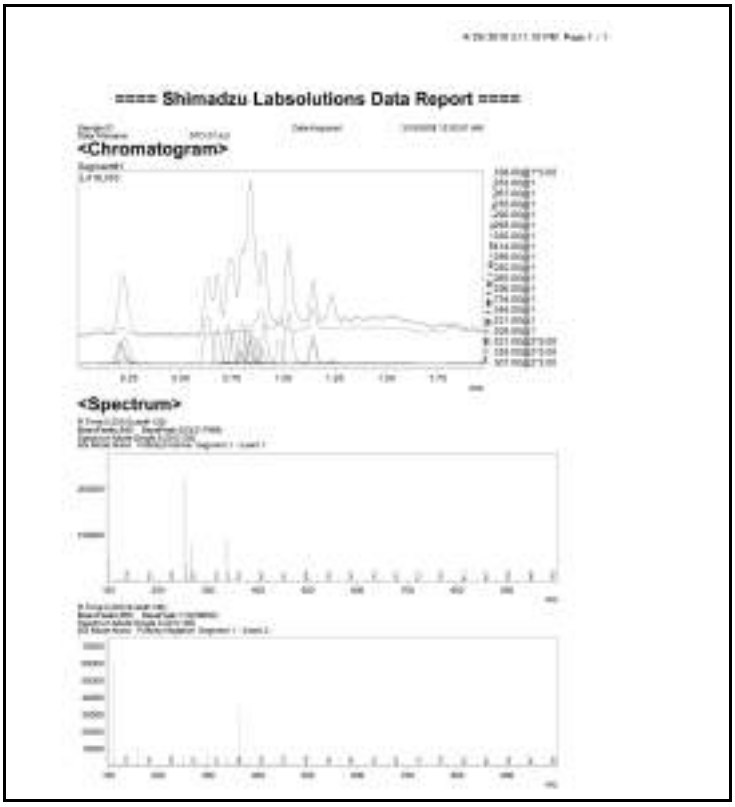
**1** **Select [Print Graph Image] on the [File] menu in the [MS Data Analysis] window, and click [Print].**



**NOTE**

The graph image can also be printed by clicking (Print) on the toolbar.

The chromatograms and spectra are printed on a single page.




## ■ Print from the Popup Menu

Select [Print Graph] from the [Chromatogram View] or [Spectrum View] right-click menu to print the chromatograms and spectra on separate pages.

This section describes how to print using the [Chromatogram View] right-click menu.

**1** **Right-click on the chromatogram in [Chromatogram View], select [Print Graph], and click [Print].**

The currently displayed chromatograms are printed on a single page.


**NOTE**

Right-click on the spectrum in [Spectrum View], select [Print Graph], and click [Print]. The currently displayed spectra are printed on a single page.

## 6.9.2 Print Using a Report Format

Data reports can be printed using the report format displayed in the [Report] window.

**1** **Click the (Data Report) icon on the [MS Data] assistant bar.**

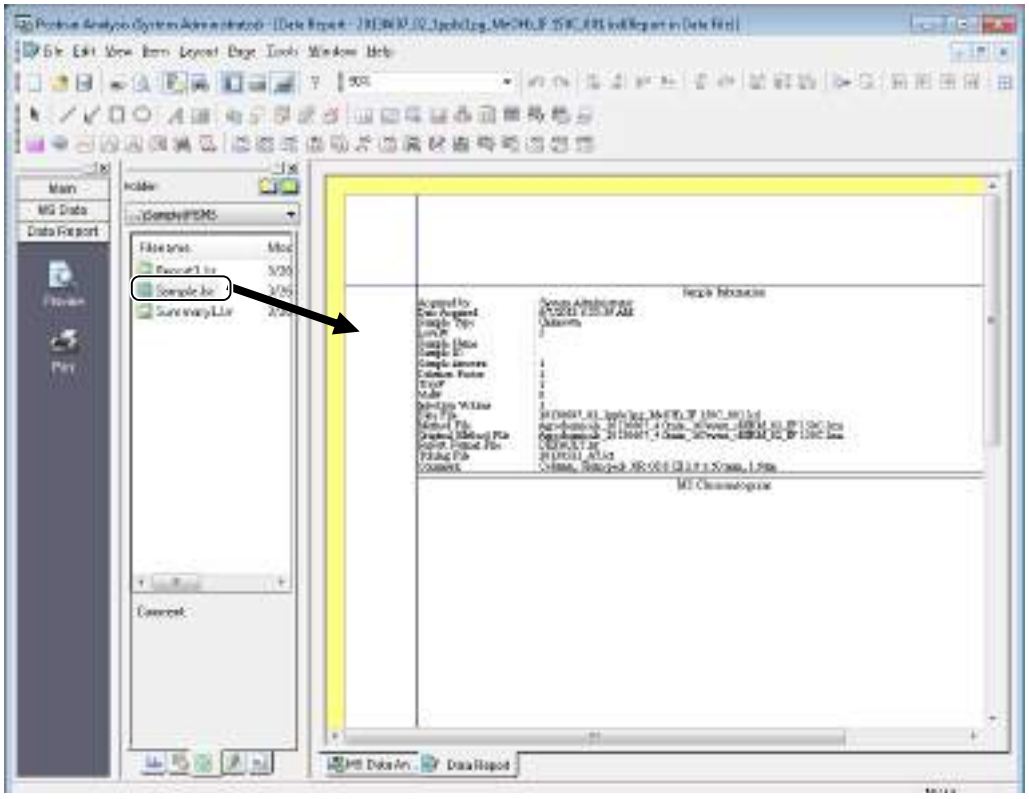
The [Report] window opens. If a report file was specified in data acquisition or postrun batch, that template is loaded.

**NOTE**

The [Report] window can also be opened by selecting [Data Report] on the [File] menu in the [MS Data Analysis] window and clicking [Edit Format].

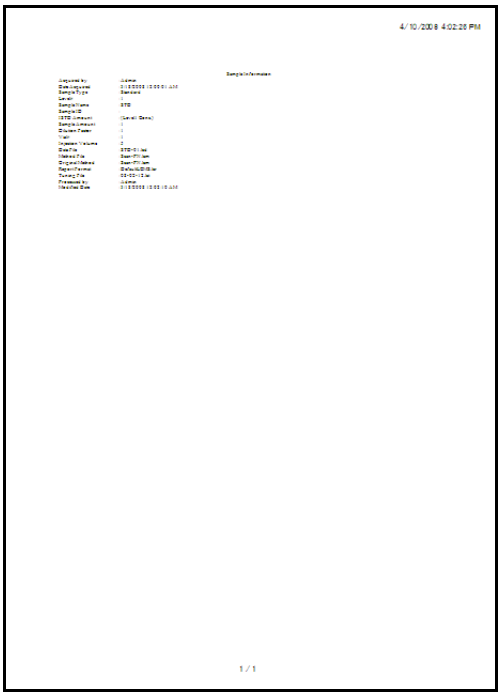
**2** **Click the [Report Format] tab in the [Data Explorer] sub-window to change the template, and drag-and-drop the desired report file onto the [Report] window.**

Select the report file “Sample1.lcr” in this example.
The report format opens.



**3** **Click the (Print) icon on the [Report] assistant bar.**

The report is printed as currently displayed in the [Report] window.



# 6.10 Use Mass Spectrum Pattern

This section describes how to check the identification results of a compound using automatic MS/MS or the (MSn) library search feature.

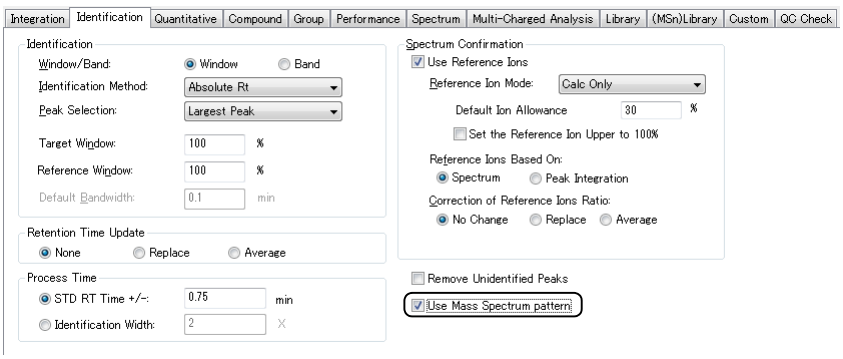
**NOTE**

One or more events set in the Compound Table must be set in the dependent event of an MRM survey event. See *"6.3.4 MS Spectrum Library Searches" P.207* for details on how to set (MSn) library search criteria.

## ■ Set Identification Conditions

**1** **Click Edit (Edit Mode) in [Method View].**

**2** **Click the [Identification] tab, and select [Use Mass Spectrum Pattern].**



**3** **Click View (View Mode) in [Method View].**

## ■ Perform Quantitative Processing on Chromatograms

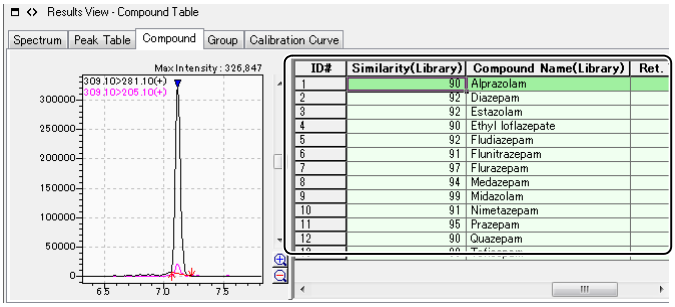
See *"6.5.2 Quantitative Processing on Chromatograms" P.220* for details on how to perform quantitative processing on chromatograms.

## ■ Check Mass Spectrum Pattern Results

Check mass spectrum pattern results in the [Compound] tab in [Results View].

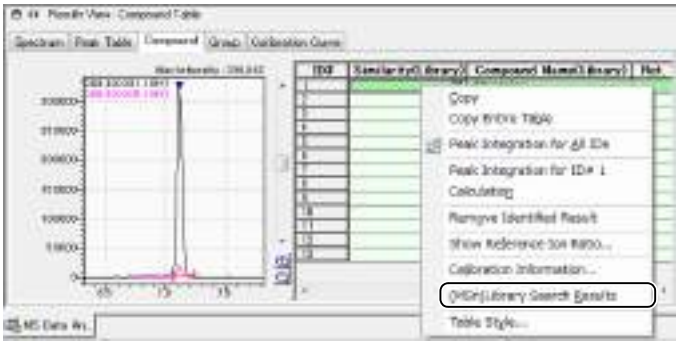
**1** **Click [Compound] tab in [Results View].**

Mass spectrum pattern results are displayed in the Compound Result Table.



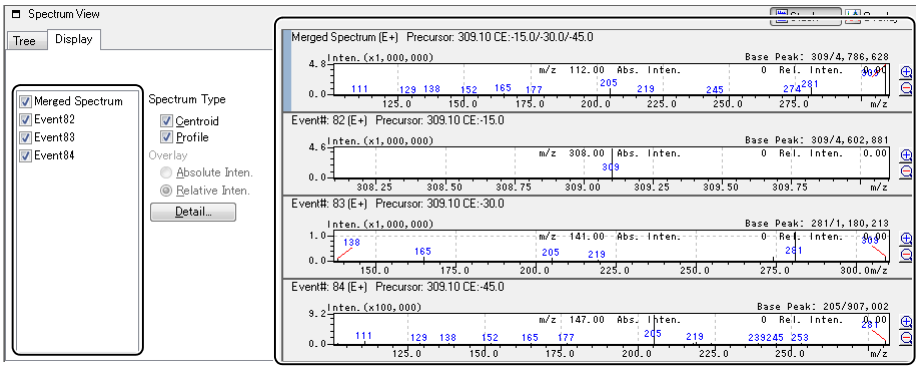

**NOTE**

If the mass spectrum pattern results are not displayed in the Compound Result Table, right-click on the Compound Result Table, select [Table Style], and add [Similarity(Library)], [Compound Name(Library)], and [Ret. Time(Library)] to the [Display Items] box.

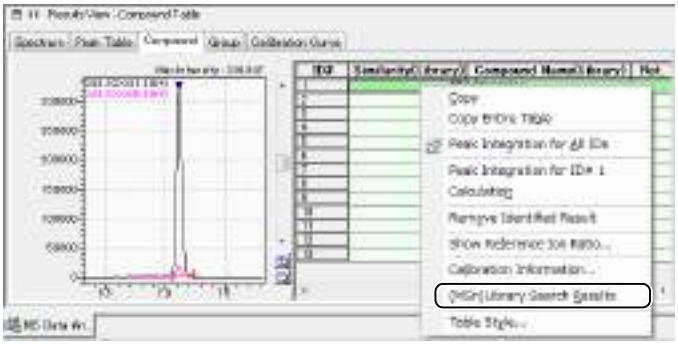


**NOTE**

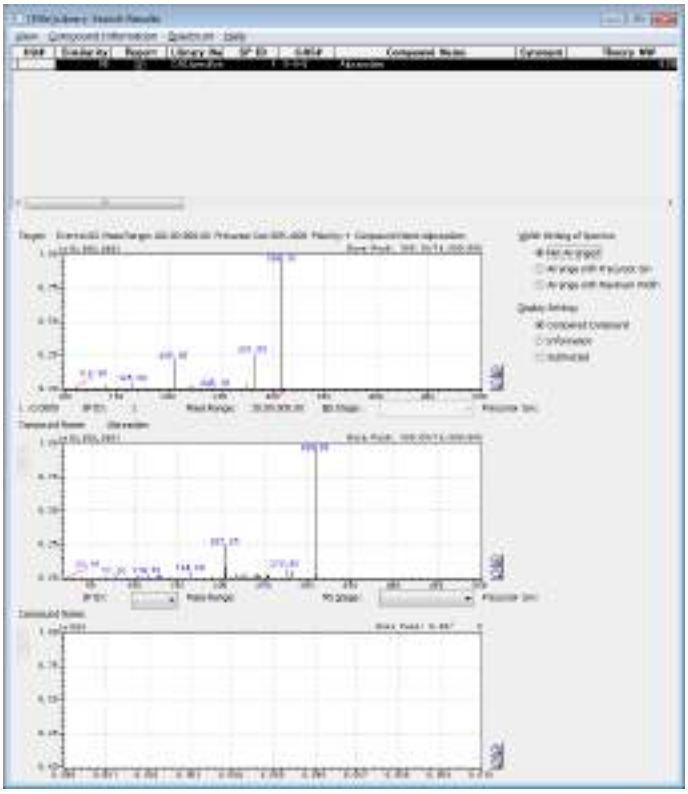
Merged Spectrum combined with the dependent event spectra related to the compound and dependent event spectra are displayed in [Spectrum View]



## 2 Right-click the row showing the mass spectrum pattern results in the Compound Result Table and click [(MSn) Library Search Results].




The [(MSn) Library Search Results] screen appears.



# 7 Report Function

This chapter describes how to use the report function to print chromatograms and quantitative results.

Use the report format function, to combine report items, such as sample information, chromatograms and quantitative results, to create reports in various formats.

## 7.1 Print Reports in Batch Processing

This section describes how to use the Batch Table to print reports in realtime batch.

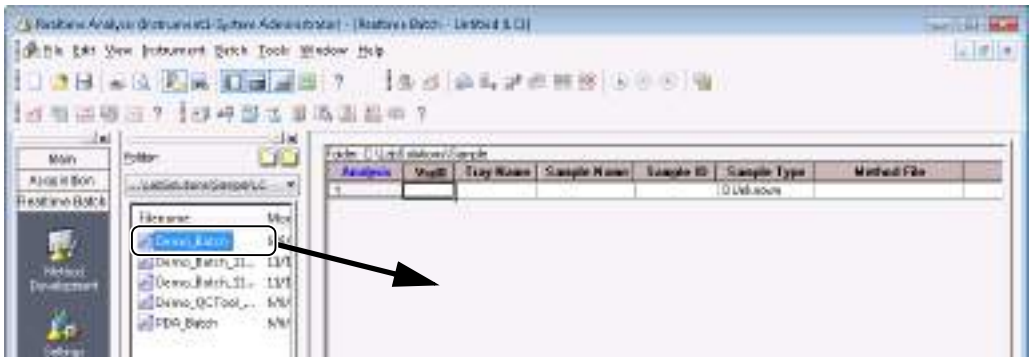
**Reference**

Refer to *"3.2 Create Batch Tables" P.43* for details on creating a new Batch Table.

**1** **Click the (Realtime Batch) icon on the [Main] assistant bar in the [Realtime Analysis] program.**

**2** **Click (Toggle Data Explorer) on the toolbar.**

**3** **In the [Data Explorer] sub-window, drag-and-drop the target batch file onto the Batch Table.**

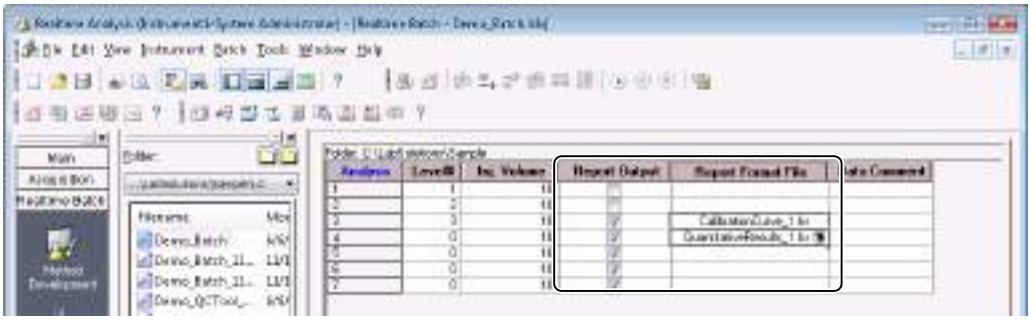


**4** **Select the [Report Output] cell in the desired rows, and select the [Report Format File].**

- If a new report format file has not been created, select an installed report format file in the [Report Format File] cell.
- If a report format file has been created, select that report format file in the [Report Format File] cell.
- If the [Report Format File] cell is left blank, the default report format file “Default.lsr” is used to print the report.

**Reference**

Refer to *"7.1.1 Change the Default Report Format File" P.246* for details on the default report format file.



**5** **Click the (Start Realtime Batch) icon on the [Realtime Batch] assistant bar.**

The report is automatically printed when data acquisition for the selected row is complete.

**NOTE**

Set the Batch Table in the same way in the [Postrun Batch] window, to automatically print reports in postrun batch.

**Reference**

Refer to *"3.4.4 Print a Summary Report" P.62* for details on outputting summary reports.

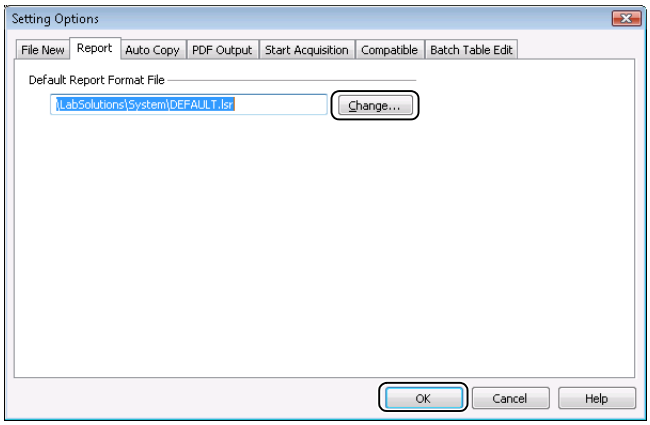
## 7.1.1 Change the Default Report Format File

When [Report Output] is selected for single run or realtime batch, reports are printed in a pre-determined default report format even if a report format file is not set.

This section describes how to change the default report format file in the [Realtime Batch] window.

**1** **Click [Options] on the [Tools] menu in the [Realtime Batch] window.**

**2** **Click [Change] on the [Report] tab, set the report file to change, and click [OK].**




**NOTE**

- Do not delete or move the default report format file.
- If the [Report Format File] cell is left blank and [Report Output] is selected, reports are printed in the report format saved in each data file.

**Reference**

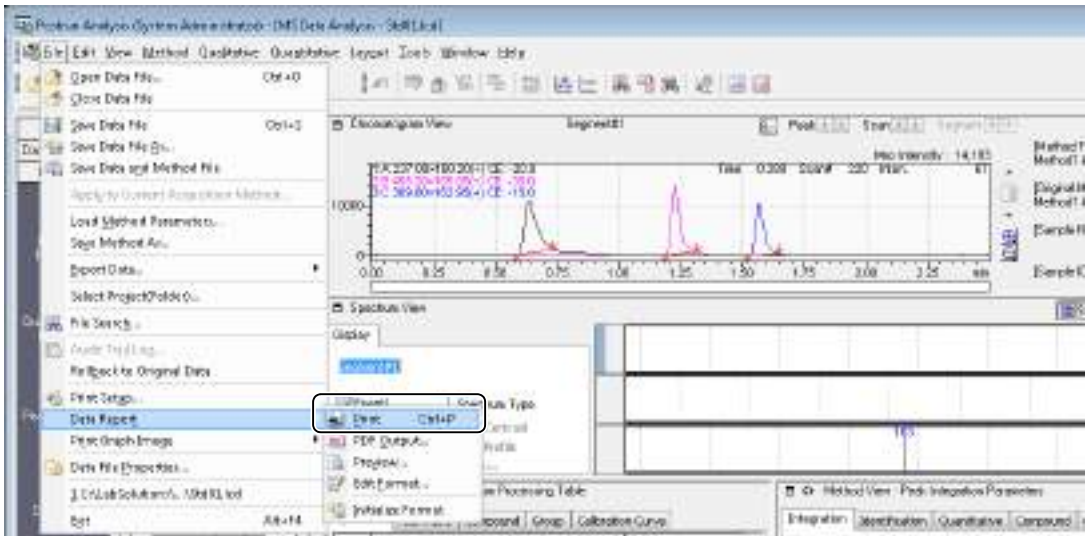
Refer to *"7.2 Print Data Processing Results" P.247* for details on the report format saved in each data file.

# 7.2 Print Data Processing Results

7

This section describes how to print reports from data files in the [Data Analysis] window or [PDA Data Analysis] window.

**1** **Open the data file in the [Data Analysis] window or [PDA Data Analysis] window, select [Data Report] on the [File] menu, and click [Print].**



The report is printed.

**NOTE**

- If a report format file was not specified at the time of data acquisition, the default report format file [Default.lsr] is used to print the report.
- Select [Data Report] on the [File] menu, and click [Preview] to check the printed details. The preview sub-window opens.
- Select [Data Report] on the [File] menu, and click [Edit Format] to change the report format. The report format in the data file is edited.

**Reference**

Refer to *"7.4 Create a Report Format File" P.253* for details on pasting new items to reports.

# 7.3 Edit Report Format Files

This section describes how to open the pre-installed report format file “peak report_1.lsr” in the [Report] window, and display the compound name in the peak top comment of the chromatogram.

**1** **Click the (Report Format) icon on the [Main] assistant bar.**

The [Report] window opens.

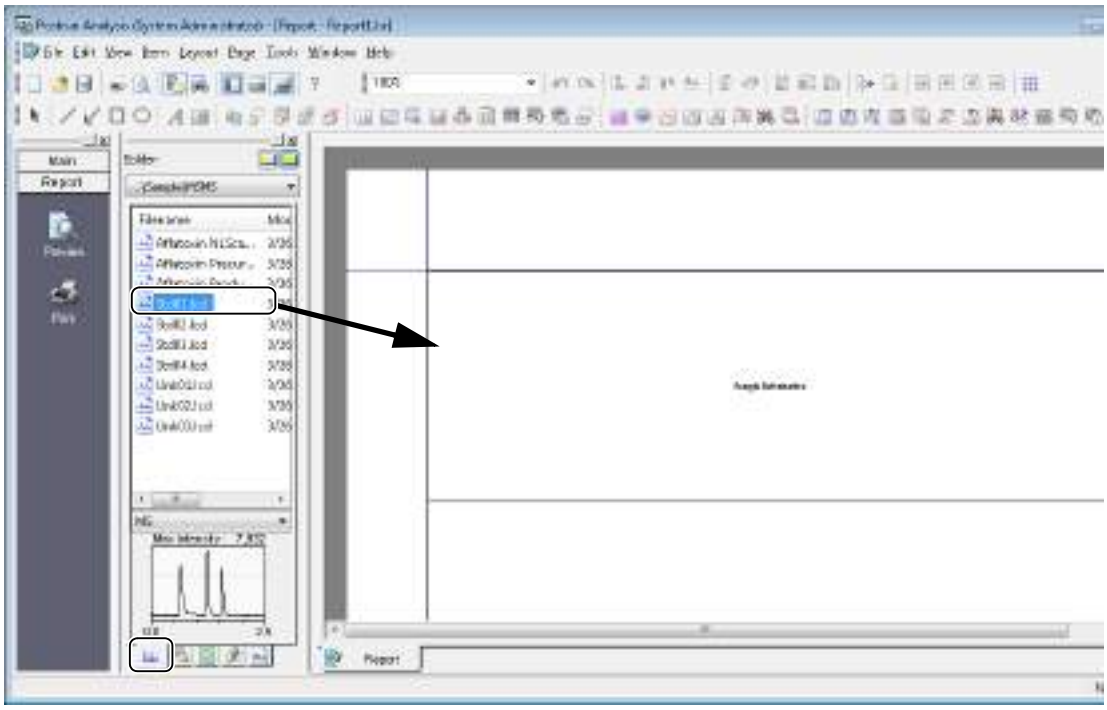
**2** **Click (Select Folder) in the [Data Explorer] sub-window.**

**3** **Select “\LabSolutions\Sample”, and click [Close].**

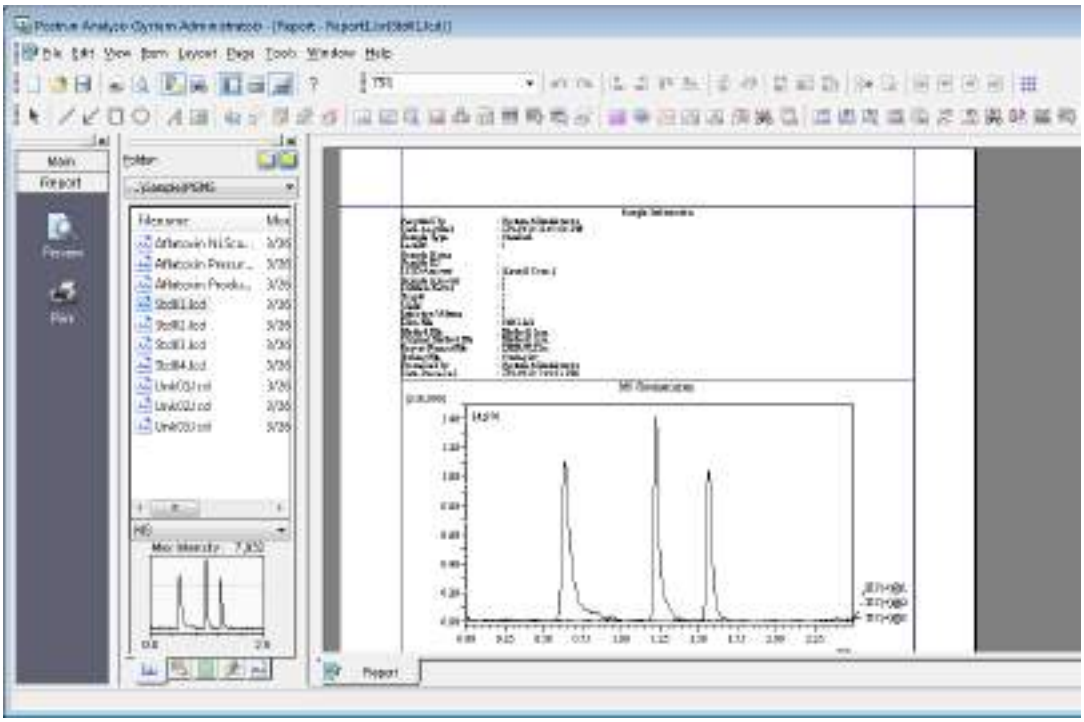
The contents of the “\LabSolutions\Sample” [Folder] is displayed in the [Data Explorer] sub-window.

**4** **Drag-and-drop “Report1.lcr” from the [Data Explorer] sub-window onto the [Report] window.**

**5** **Click the (Data) tab at the bottom of the [Data Explorer] sub-window, and drag-and-drop the data file.**



The contents of the data file is displayed in the [Report] window.



**NOTE**

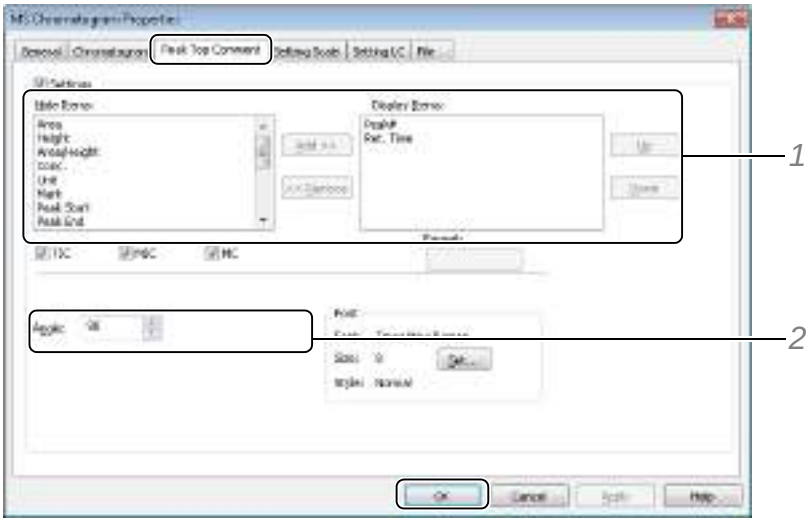
If the data file is not displayed in the [Data Explorer] sub-window, click (Select Folder), and specify the folder that contains the desired data file.

**6** **Double-click the chromatogram item.**

The [Chromatogram Properties] sub-window opens.

**7** **Click the [Peak Top Comment] tab, enter the [Chromatogram] tab parameters.**

**8** **Click the [Peak Top Comment] tab, enter the [Peak Top Comment] tab parameters, and click [OK].**




*1* Select [Name] in the [Hide Items] box, and click [Add].
[Name] is displayed in the [Display Items] box.

**NOTE**
Click [Format] to open the [Format Settings] sub-window to edit the number of display digits and rounding method. Refer to *"7.5.8 Edit the Numeric Value Format in the Quantitative Results Table" P.265* for details.

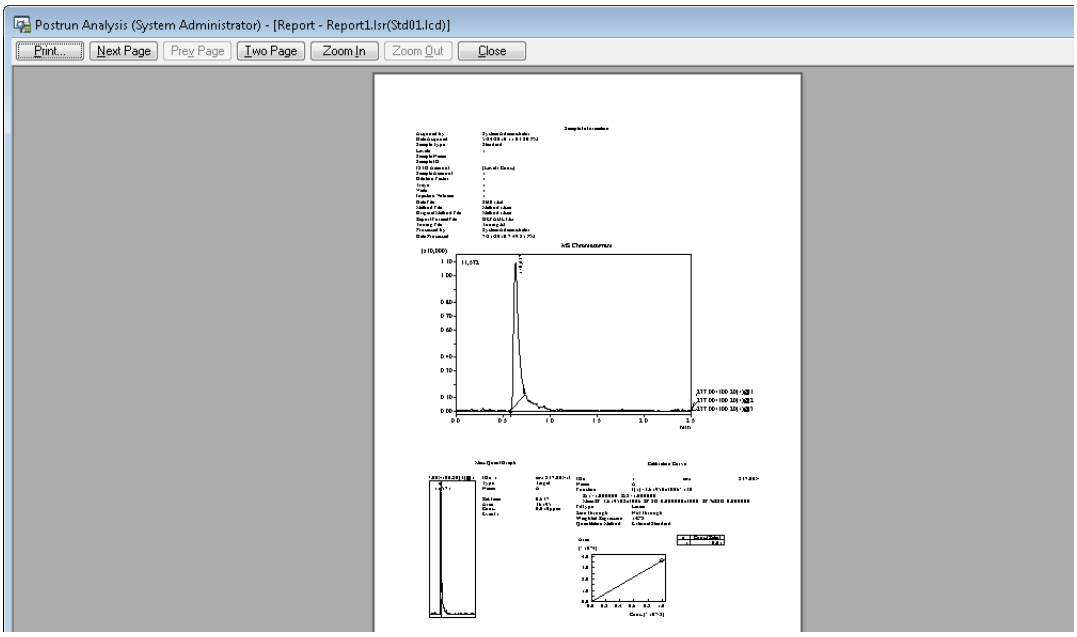
*2* Enter the [Angle] to change the angle or position of the peak top comment.

**NOTE**
The default angle is “90”. Increase the value to rotate the comment counterclockwise from the start of the text string.

**Reference**
Refer to *"7.4 Create a Report Format File" P.253* for details on adding items to the report format.
Refer to *"7.5 Edit Report Items" P.258* or *"5.7.3 Edit PDA Report Format" P.163* to edit other report format items.

**9** **Click the (Preview) icon on the [Report] assistant bar.**

## 10 Preview the report, and click [Close].




## 11 Click [Save Report Format File As] on the [File] menu.

## 12 Enter a file name at [Save in], and click [Save].

# 7.4 Create a Report Format File

This section describes an example of how to make a new report format file in the [Report] window.

**Reference**

Refer to *"7.5 Edit Report Items" P.258* for details.

**1** **Click the (Report Format) icon on the [Main] assistant bar.**

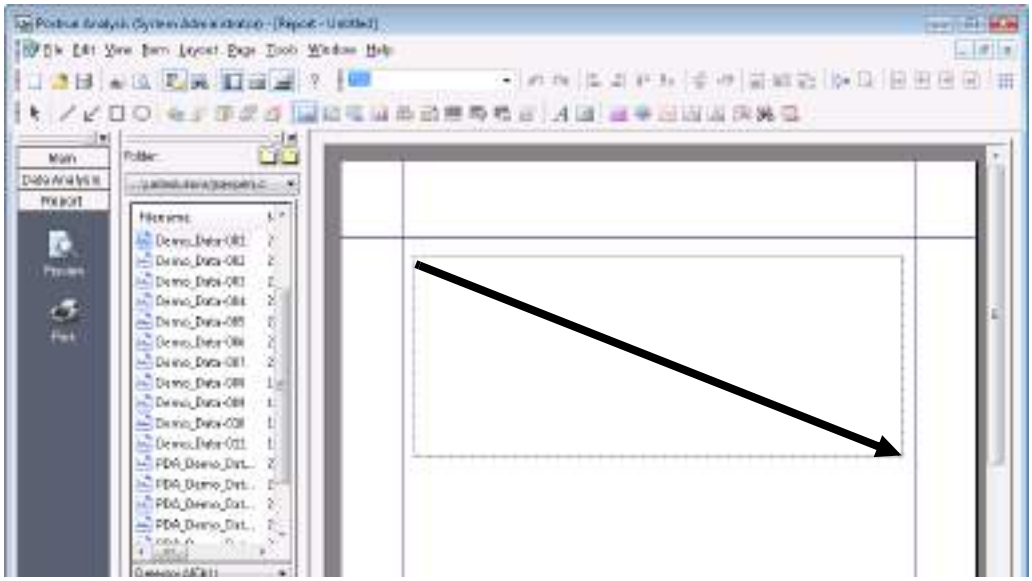
**2** **Click (New) on the toolbar.**

**3** **Click (Chromatogram) on the toolbar.**

**Reference**

Refer to *"7.4.1 Types of Report Items" P.256* for details on each toolbar item.

**4** **Drag the cursor on the format to specify a range for the chromatogram.**



**5** **In the [LC/PDA Chromatogram Properties] sub-window, correct the display position and edit the display items, and click [OK].**

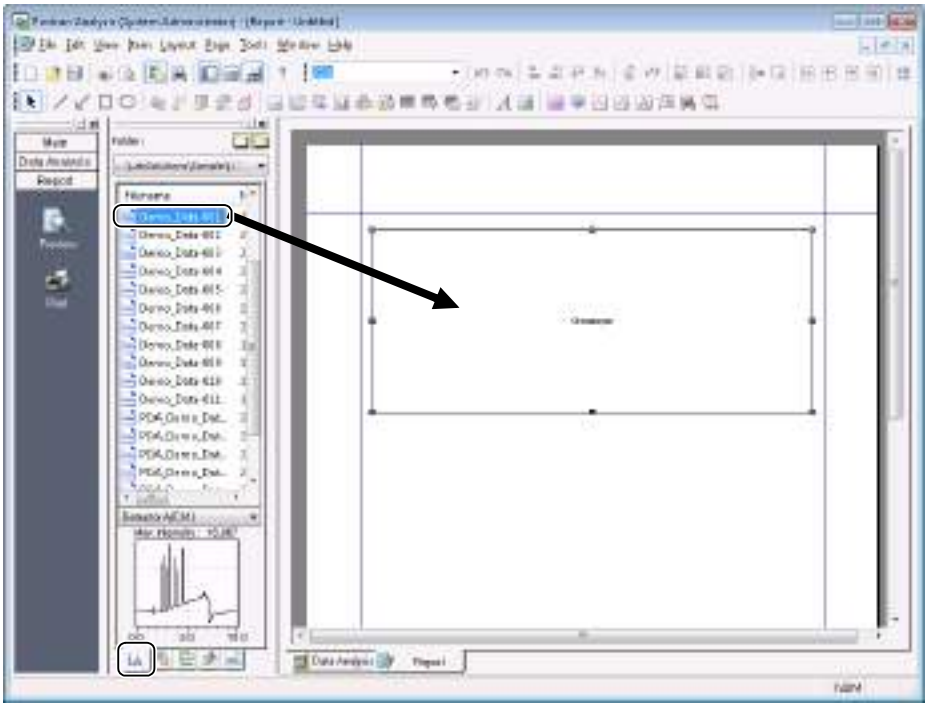
**NOTE**

Double-click inside the item frame to open the [LC/PDA Chromatogram Properties] sub-window.

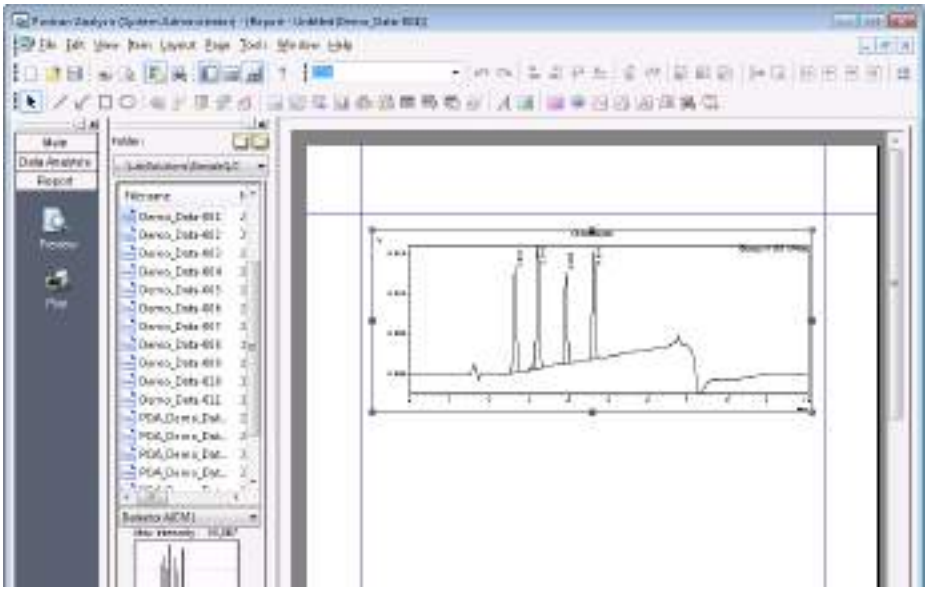
**Reference**

Refer to *"7.5.1 Chromatogram Properties" P.258* or *"7.5.2 Change the Chromatogram Display Scale" P.259* for details on editing the chromatogram display.

**6** **Click the (Data) tab at the bottom of the [Data Explorer] sub-window and drag-and-drop the target data file onto the report format to examine the print details of a report format file.**



The chromatogram information of the data file is displayed in the [Report] window.



**NOTE**

- Right-click on an item and click [Delete] to remove the item.
- Drag-and-drop the data file to a specific item with the [Shift] key held down to load data only to that item.
- If the data file is not displayed in the [Data Explorer] sub-window, click (Select Folder), and specify the folder containing the desired data file.

**7** **Click the (Preview) icon on the [Report] assistant bar.**

**8** **Examine the report in the preview sub-window, and click [Close].**

**9** **Click [Save Report Format File As] on the [File] menu.**

**10** **Specify a folder at [Save in], enter a [File Name], and click [Save].**

## 7.4.1 Types of Report Items

Items, such as chromatograms and quantitative result information, can be added to the report format using the icons on the toolbar. The following report items are available.

| Item | Content |
|---|---|
| Figure | Use these icons to add a Line, Arrow, Rectangle or Ellipse to the report format. |
| Text | Use this icon to add a text box to the report format. |
| Picture | Use this icon to add bitmaps or other image files to the report format. |
| System Configuration | Use this icon to add the instrument configuration at the time of data acquisition to the report format. |
| Sample Information | Use this icon to add sample information to the report format. |
| Method | Use this icon to add method file information, such as the instrument and data processing parameters to the report format. |
| Batch Table | Use this icon to add the Batch Table and batch file settings to the report format. |
| System Check | Use this icon to add the system check results saved in data files to the report format. |
| Chromatogram | Use this icon to add chromatograms and instrument status information to the report format. |
| Calibration Curve | Use this icon to add the calibration curve graph and information to the report format. |
| Peak Table | Use this icon to add a table of the retention times and area values of detected peaks to the report format. |
| Quantitative Results | Use this icon to add a table of the quantitative results of identified peaks to the report format. |
| Group Results | Use this icon to add a table of the quantitative results for grouped compounds to the report format. |
| Fraction Collection Report | Use this icon to add a table of the fraction collection status to the report format. |
| Summary (Concentration) | Use this icon to add a summary of the chromatograms, statistical concentration results, areas and heights for multiple data acquisitions to the report format. |
| Summary (Compound) | Use this icon to add a summary of the concentrations, areas and heights of multiple data by individual compound to the report format. |
| Summary (Data) | Use this icon to add a summary of the chromatograms and Peak Tables for multiple data to the report format. |
| Contour Graph | Use this icon to add contour graphs of PDA data to the report format. |
| 3D Graph | Use this icon to add 3D graphs of PDA data to the report format. |
| UV Spectrum | Use this item to add PDA spectra and spectra information to the report format. |
| Peak Purity | Use this icon to add the PDA peak purity results to the report format. |
| Peak Profile | Use this icon to add the PDA peak profile information to the report format. |
| UV Spectrum Index | Use this icon to add PDA chromatograms and spectra for detected peaks to the report format. |
| UV Library Search | Use this icon to add UV Library Search results to the report format. |
| UV Library | Use this icon to add a list of the spectra in the library file to the report format. |

| Item | Content |
|---|---|
| MS Chromatogram | Use this icon to add the MS chromatograms to the report format. |
| MS Calibration Curve | Use this icon to add the MS calibration curve graph and information to the report format. |
| MS Peak Table | Use this icon to add a table of the retention times and area values for the detected MS peaks to the report format. |
| MS Quantitative Graph | Use this icon to add MS chromatograms for identified peaks to the report format. |
| MS Quantitative Table | Use this icon to add a table of MS quantitative results for identified peaks to the report format. |
| MS Spectrum | Use this icon to add the MS spectrum information to the report format. |
| MS Library Search | Use this icon to add the MS Library Search results to the report format. |
| MS Status Log | Use this icon to add the MS instrument status to the report format. |
| MS Summary (Concentration) | Use this icon to add a summary chromatograms, statistical concentration results, areas and heights for multiple MS data acquisitions to the report format. |
| MS Summary (Compound) | Use this icon to add a summary of the concentrations, areas and heights of multiple MS data by individual compound to the report format. |
| MS Summary (Data) | Use this icon to add a summary of the chromatograms and Peak Tables for multiple MS data to the report format. |
| LC/MS/MS Tuning | Use this icon to add the LCMS-8030/8040/8045/8050/8060 tuning results to the report format. |
| MS Quantitative Result(Mass Spectrum Pattern) | When the mass spectrum pattern is used in the identification, the chromatograms and quantitative results for identified peaks and the pattern matching results are displayed. Automatic MS/MS data in LCMS-8030/8040/8045/8050/8060 is used for pattern matching. |

# 7.5 Edit Report Items

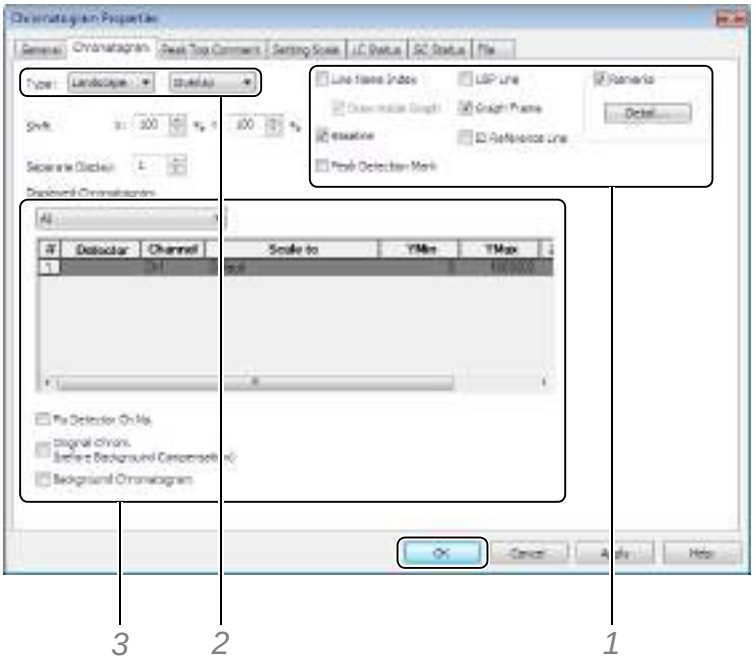
This section describes how to edit properties for each report item.

## 7.5.1 Chromatogram Properties

The following section describes how to set the chromatogram display properties on the [Chromatogram] tab of the [Chromatogram Properties] sub-window.

**1** **Click the [Chromatogram] tab.**

**2** **Enter the properties on the [Chromatogram] tab, and click [OK].**




1 Select each of the checkboxes to print the [Baseline] and [Peak Detection Mark].

2 Click [Portrait] and [Overlay] in the [Type] list to draw chromatograms overlaid in a portrait orientation.
Click [Landscape] and [Separate] in the [Type] list to draw chromatograms overlaid in a landscape orientation.

3 Click [All] in the [Displayed Chromatogram] list.

**NOTE**

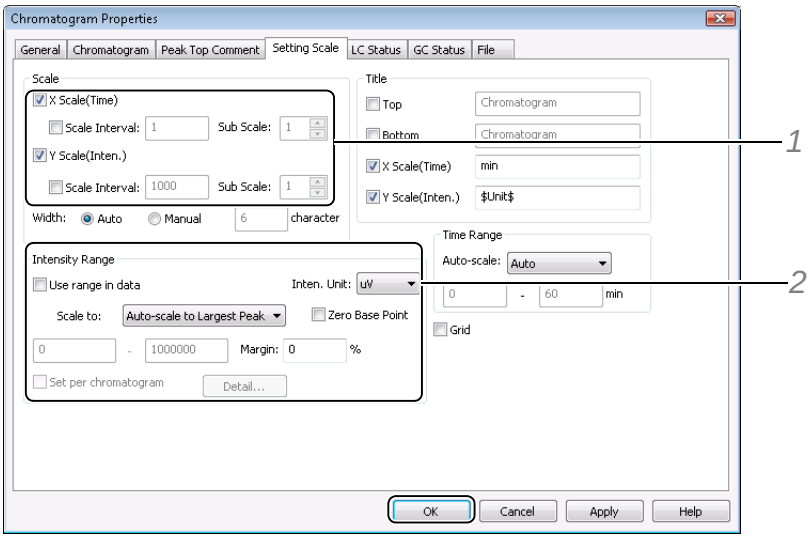
- When [Select Chromatogram] in the [Displayed Chromatogram] list is selected and select the detector in [Detector], all of the channels set by that detector are displayed.
- When [No Chromatogram] is selected in the [Displayed Chromatogram] list, chromatograms are not displayed. Use this parameter to display only the instrument status.

## 7.5.2 Change the Chromatogram Display Scale

Set the chromatogram display scale and scale interval on the [Setting Scale] tab of the [Chromatogram Properties] sub-window. The scale of the intensity axis can also be changed for each chromatogram.

**1** **Click the [Setting Scale] tab.**

**2** **Enter the [Setting Scale] tab parameters, and click [OK].**




*1* Select [Scale Interval], and set the interval at [Scale Interval] and [Sub Scale] to display the scale on the intensity axis (Y-axis) and time axis (X-axis).

*2* Deselect [Use range in data], and select the display unit and reference peak at [Inten. Unit] and [Scale to] to set the chromatogram intensity axis (Y-axis).

**NOTE**

- The default setting is [Use range in data], and the intensity unit and intensity axis range saved in data files are used.
- If [Zero Base Point] is selected and a setting other than [User Defined] is selected at [Scale to], chromatograms are auto-scaled and displayed on the intensity axis of 0 V or more.
- Set the upper/lower width (margin) of the intensity axis at [Margin] when chromatogram displays are auto-scaled.
- If the intensity axis is unique for each chromatogram, for example, because the peak height of obtained by data acquisition differs for each detection channel, select [Set per Chromatogram] and enter the upper limit and lower limit values for each chromatogram.

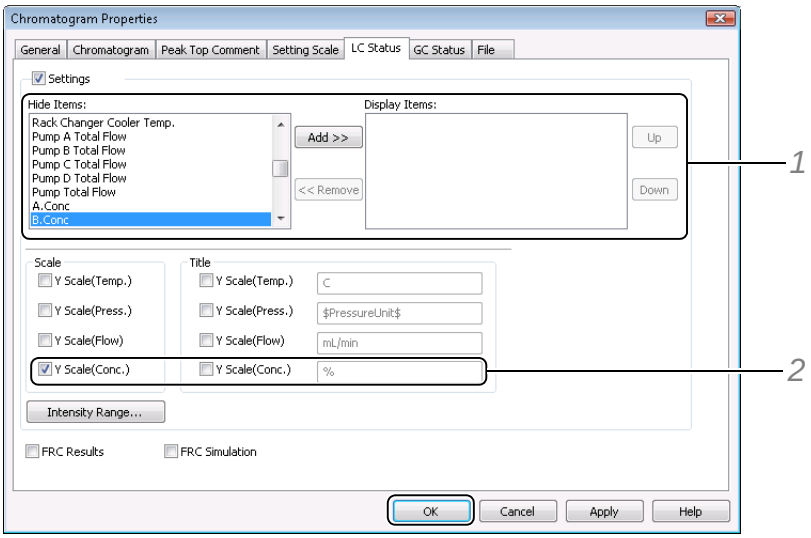
## 7.5.3 Display the Instrument Status and Gradient Curve

Use the [LC Status] tab of the [Chromatogram Properties] sub-window to overlay the instrument status information and gradient curve on chromatograms.

This section describes how to overlay the gradient curve for pump B (B.Conc%) on a chromatogram.

**1** **Click the [LC Status] tab.**

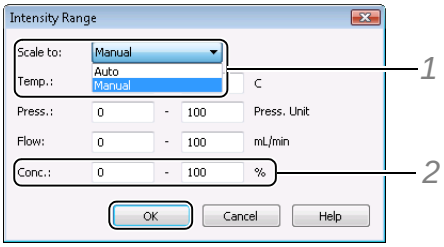
**2** **Enter the [LC Status] tab parameters, and click [OK].**




*1* Select [B.Conc] in the [Hide Items] box, and click [Add].
[B.Conc] is added to the [Display Items] box.

*2* Select [Y Scale (Conc.)] at [Scale] and [Title].

**3** **Click [Intensity Range] to set the intensity axis range.**




*1* Click [Manual] in the [Scale to] list.

*2* Enter the upper limit and lower limits at [Conc].

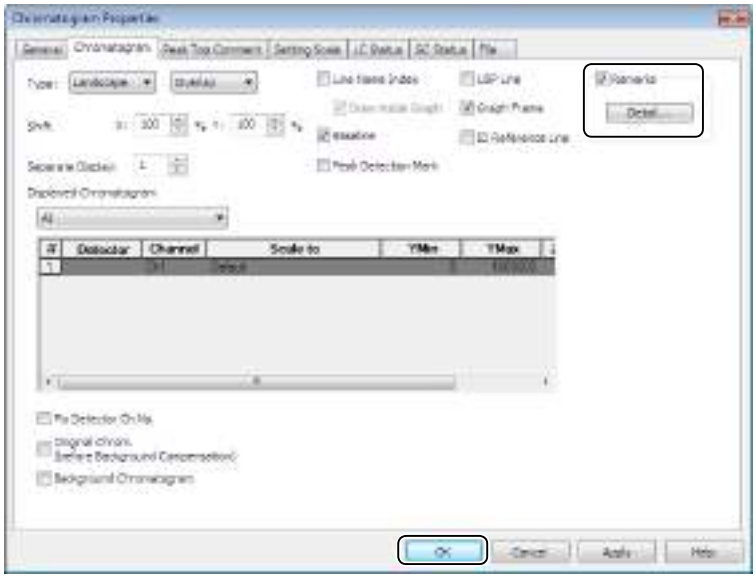
*3* Click [OK].

**4** **Check the edited details, and click [OK].**

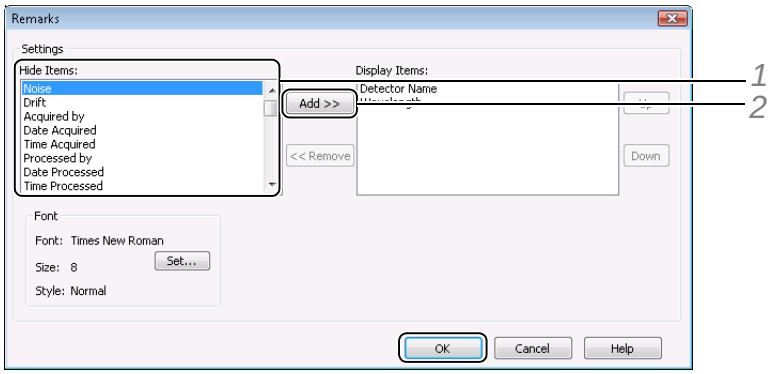
## 7.5.4 Edit Sample Information Display

Click [Remarks] on the [Chromatogram] tab of the [Chromatogram Properties] sub-window, and select the desired remark to display sample information in the chromatogram remarks section.

**1** **Click the [Chromatogram] tab, select [Remarks], and click [Detail].**



**2** **Select the display item in the [Remarks] sub-window, and click [OK].**




*1* Select the items to print in the [Hide Items] box.

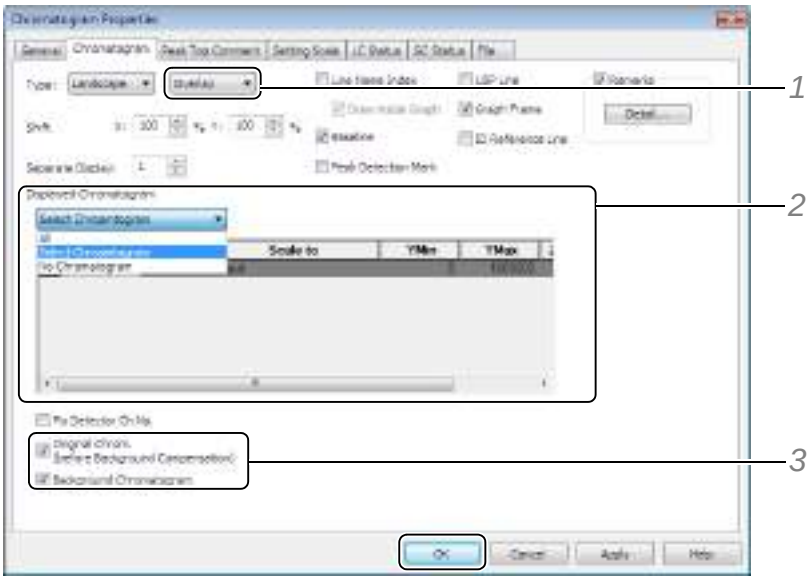
*2* Click [Add].
The added items are displayed in the [Display Items] box.

## 7.5.5 Display the Background File

Use the [Chromatogram] tab in the [Chromatogram Properties] sub-window to overlay the background data or the chromatograms before background compensation.

**1** **Click the [Chromatogram] tab.**

**2** **Enter the [Chromatogram] tab parameters, and click [OK].**



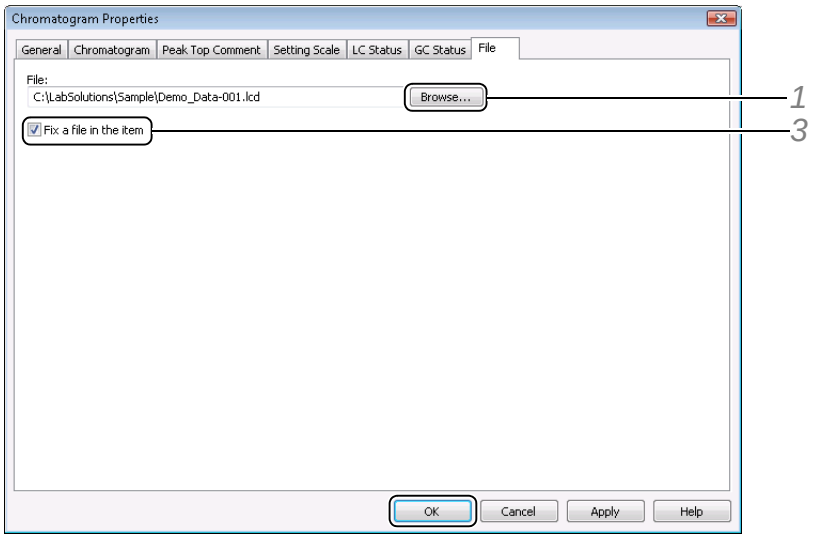

1 Click [Overlay] in the [Type] list.
2 Select the checkbox of the chromatograms to be overlaid at [Displayed Chromatogram].
3 Select [Original Chrom. (before Background Compensation)] and [Background Chromatogram].

## 7.5.6 Attach a Specific Chromatogram to the Report Format

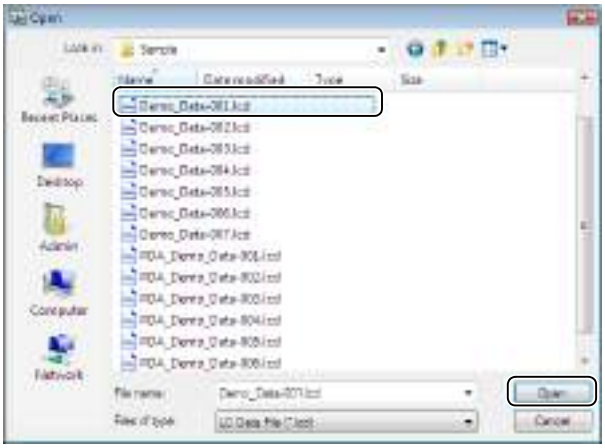
Enter a file on the [File] tab of the [Chromatogram Properties] sub-window to attach a specific (reference) chromatogram to the report format and cause the same chromatogram to be printed each time the report format is used to print data.

**1** **Click the [File] tab.**

**2** **Select the [File] tab parameters, and click [OK].**




*1* Click [Browse] and select the desired data file, and click [Open].




*2* Select [Fix file in the item].

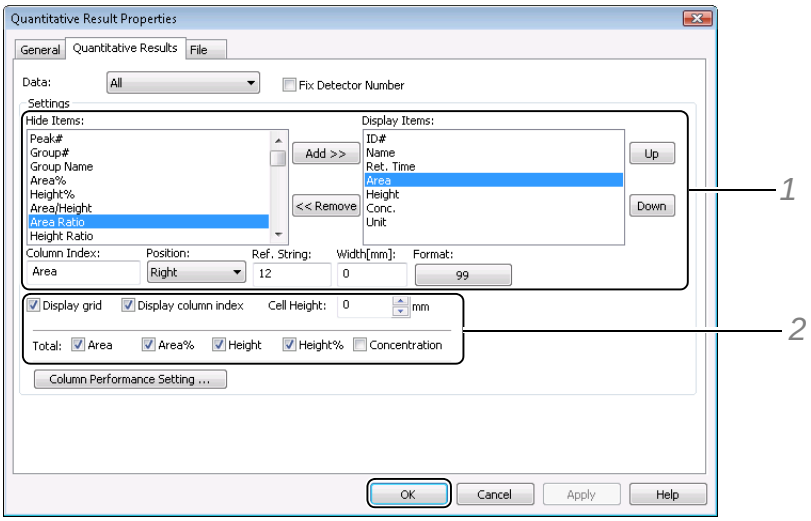
**NOTE**

Select [Fix file in the item] to print the chromatogram selected in [File] each time the report format is used. This selected chromatogram is printed even if a different data file is loaded in the [Report] window.

## 7.5.7 Edit the Quantitative Results Table

**1** **Click the [Quantitative Results] tab.**

**2** **Set the [Quantitative Results] tab parameters, and click [OK].**




*1* Select items to print in the [Hide Items] box, and click [Add].
The added items are displayed in the [Display Items] box.

*2* Select the desired items to display statistical calculation results and the grid.

**NOTE**

When displayed items include column performance parameters (e.g. number of theoretical plates and tailing factor), all values calculated by the various pharmacopoeia methods (JP, USP, etc.) specified in the data processing parameters are displayed.
To filter the reported calculation results in the Quantitative Results Table, click the [Column Performance Settings] button, select [Display only selected calc. method] in the [Display Settings for Column Performance Results] sub-window that is displayed, and specify the calculation results to display.

## 7.5.8 Edit the Numeric Value Format in the Quantitative Results Table

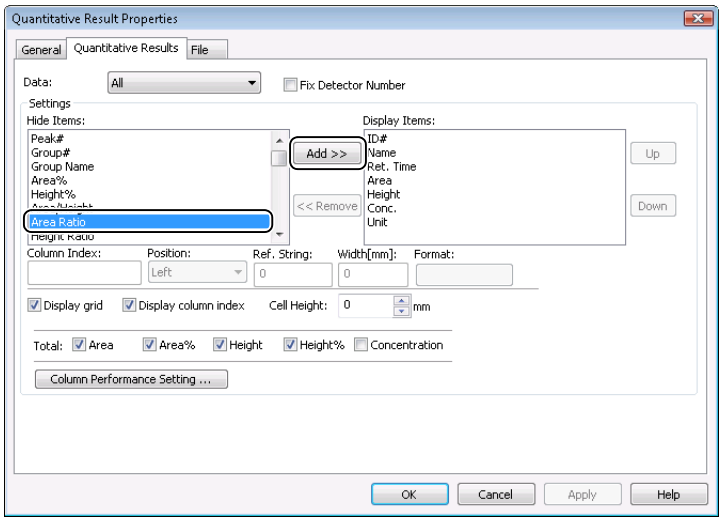
It is possible to set the rounding method and the display parameters for the numeric data.

This section describes the procedure for changing the numeric format of [Area Ratio].

**1** **Click the [Quantitative Results] tab.**

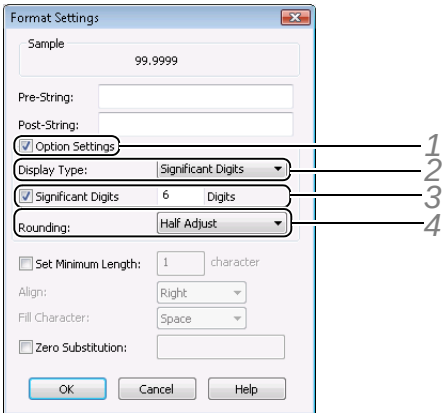
**2** **Select [Area Ratio] in the [Hide Items] box, and click [Add].**

[Area Ratio] is displayed in the [Display Items] box.




**3** **Select [Area Ratio] in the [Display Items] box, and click the [99.9999] format.**

**4** **Make the appropriate settings in the [Format Settings] sub-window, and click [OK].**




*1* Select [Option Settings].
*2* Click [Significant Digits] at [Display Type].
*3* Select [Significant Digits], and enter “6”.
*4* Click [Half Adjust] at [Rounding].

**NOTE**

By default, [Option Settings] is deselected and the display format and rounding method set in the [Data Processing Setting] sub-window for [System Settings] in [Administration Tools] are used.

**5** **Check the edited details, and click [OK].**

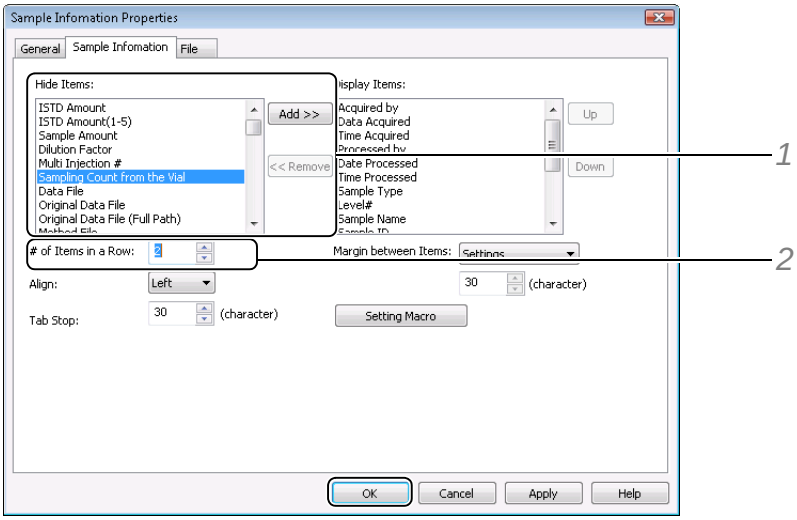
## 7.5.9 Edit Sample Information

Use the [Sample Information] tab of the [Sample Information Properties] sub-window to select the sample information to include in the report format.

The following section describes how to display the repeat injection count of the same vial number set in the batch file.

**1** **Click the [Sample Information] tab.**

**2** **Set the [Sample Information] tab parameters, and click [OK].**




*1* Select [Sampling Count from the Vial] in the [Hide Items] box, and click [Add].
[Sampling Count from the Vial] is displayed in the [Display Items] box.

*2* To display 2 sample information items in a row, enter “2” at [# of Items in a Row].

**NOTE**

Click [Setting Macro] on the [Sample Information] tab and create a method using macros to display sample information. Select the information to be displayed and the position in the macros sub-window. Once macros have been used to set the [Sample Information] tab parameters, the original table format sub-window cannot be displayed.

## 7.5.10 Edit Calibration Curve Information

Use the [Header] tab in the [Calibration Curve Properties] sub-window to edit calibration curve information such as, calibration curve expressions and quantitative calculation methods.

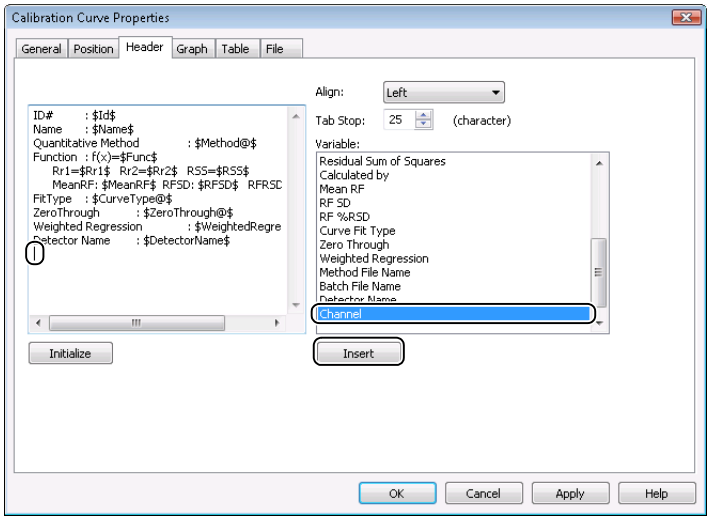
Macros are provided for each of the [Header] tab items. These macros can be edited to determine display items and positions in reports.

This section describes how to edit the [Channel] macro to print the channel.

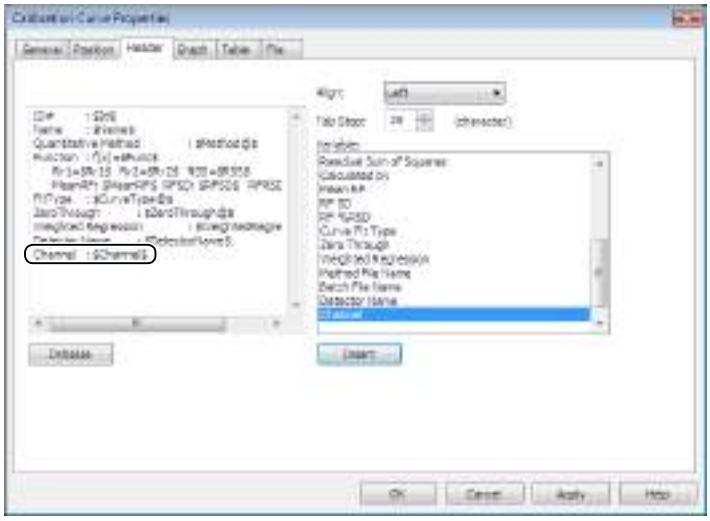
**1** **Click the [Header] tab.**

**2** **Place the cursor in the position where the new information is to be added in the display area to the left, select [Channel] in the [Variable] list, and click [Insert].**

[$Channel$] is added to the text display area.

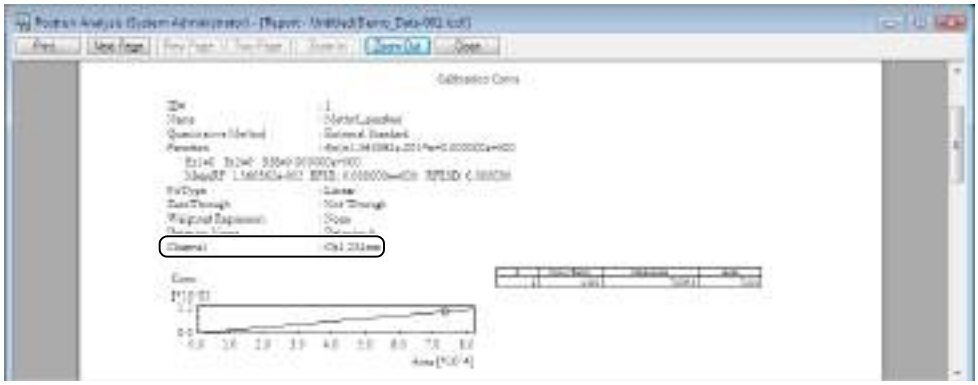



**3** **Prefix the additional macro [$Channel$] with “Channel:”.**



**NOTE**

- Tabs can be inserted by pressing the [Ctrl] and [I] keys at the same time. The tab interval is the number of characters set at [Tab Stop].
- Click [Initialize] to restore the default settings.
- Use the [Position] tab to change the display position of the calibration curve graph and table.
- [Channel] is displayed as follows:



**4** **Check the edited details, and click [OK].**

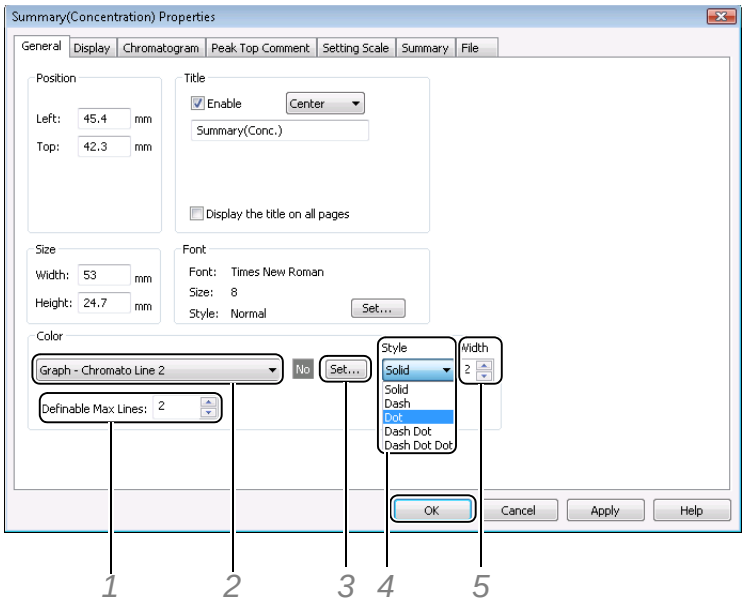
# 7.5.11 Change the Color and Line Width of Overlaid Chromatograms

Select the number of lines, line color and line width for overlaid chromatograms on the [General] tab in the [Summary (Concentration) Properties] sub-window.

This section describes how to change the color, line type and line width of overlaid chromatograms.

**1** **Click the [General] tab.**

**2** **Set the [General] tab parameters, and click [OK].**



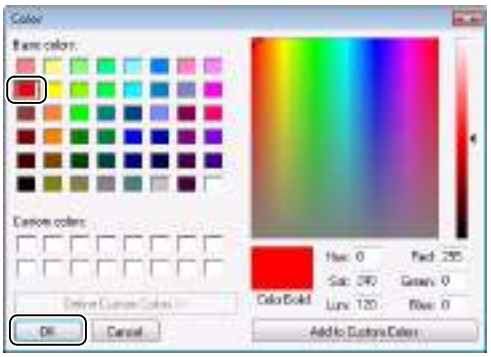

*1* Enter “2” at [Definable Max Lines].

**NOTE**

When “2” is set to [Definable Max Lines], [Graph - Chromato Line 2] is added to the [Color] list. Values higher than 2 for [Definable Max Lines] add additional chromatograms to the color list.

*2* Select [Graph - Chromato Line 2] in the [Color] list.

*3* Click [Set], select red in the [Color] sub-window, and click [OK].




*4* Click [Dot] in the [Style] list.

*5* Set [Width] to “2”.

**NOTE**

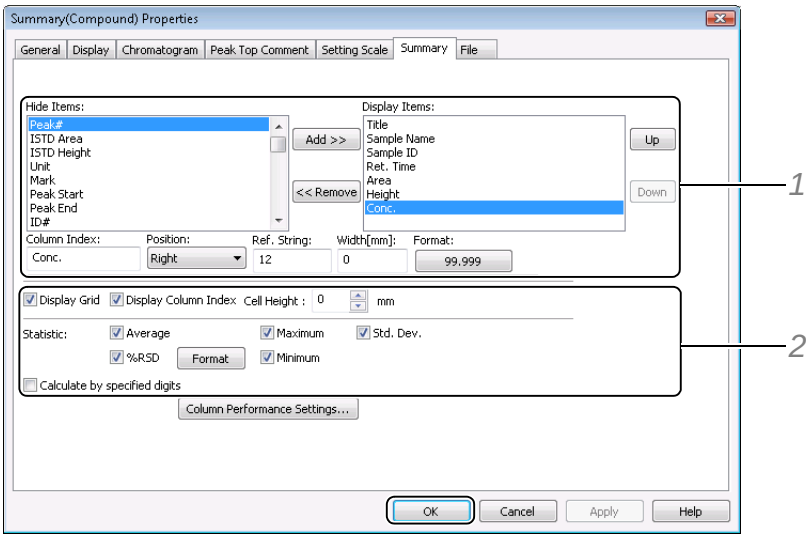
In addition to chromatograms, statistical results can also be output with the [Summary (Concentration)] item. Select the summary data (area, height and concentration) and the statistical items to display on the [Summary] tab to display the statistical calculation results of multiple data.

## 7.5.12 Edit the Statistical Results Table

Items such as statistical results can be displayed by adding them to the [Display Items] box on the [Summary] tab in [Summary (Compound) Properties].

**1** **Click the [Summary] tab.**

**2** **Set the [Summary] tab parameters, and click [OK].**




*1* Select the items to be displayed in the report in the [Hide Items] box, and click [Add].
The added items are displayed in the [Display Items] box.

*2* Select the respective items to display the statistical results and the grid in the table.

**NOTE**

- If [Calculate by specified digits] is selected, statistical calculation is performed using the number of digits set in the [Format Settings] sub-window.
- If the number of theoretical plates and tailing factor display items are selected, all values calculated by the formulas (JP method and USP method) specified in the data processing parameters are displayed.
  Click the [Column Performance Settings] button, and select [Display only selected calc. method] in the [Display Settings for Column Performance Results] sub-window to select calculation results to display in the Quantitative Results Table.

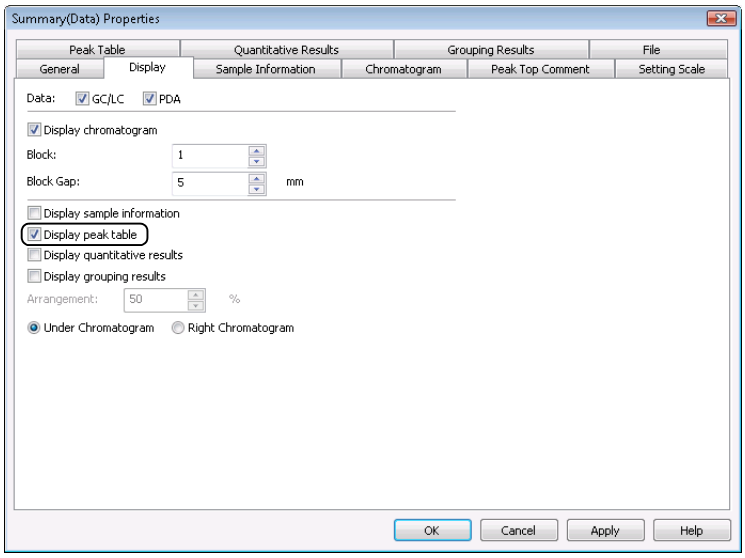
## 7.5.13 Edit the Measurement Results Table

Use the [Summary (Data)] item to display one of three tables, the Peak Table, Quantitative Results Table and Grouping Results Table.

This section describes how to use the [Summary (Data)] item to edit the Peak Table display items.

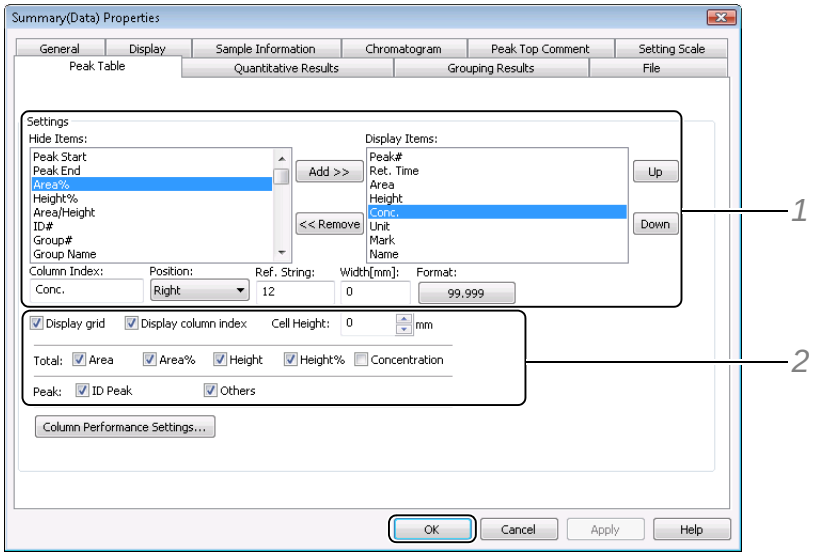
**1** **Click the [Display] tab.**

## 2 Select [Display peak table].




## 3 Click the [Peak Table] tab.

## 4 Set the [Peak Table] tab parameters, and click [OK].




*1* Select the desired items in the [Hide Items] box, and click [Add].
The added items are displayed in the [Display Items] box.

*2* Select the respective items to display the total values and grids.

**NOTE**

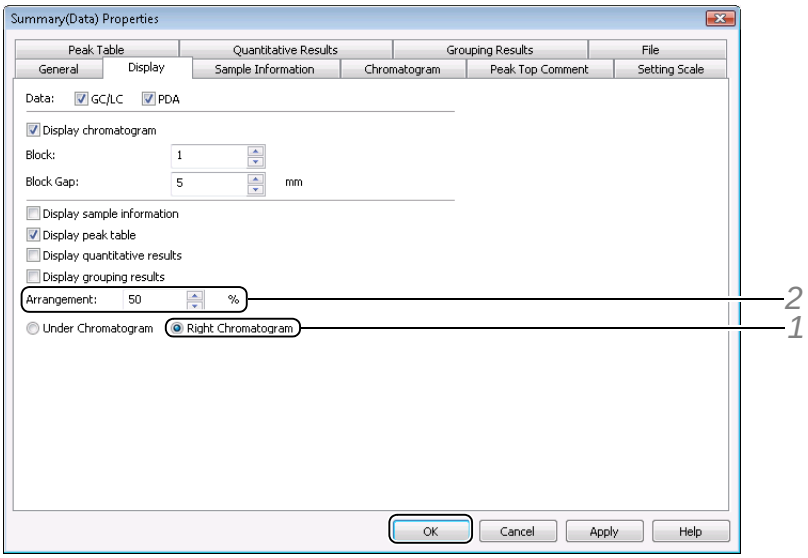
- If the number of theoretical plates and tailing factor display items are selected, all values calculated by the formulas (JP method and USP method) specified in the data processing parameters are displayed.
  Click the [Column Performance Settings] button, and select [Display only selected calc. method] in the [Display Settings for Column Performance Results] sub-window to select the calculation results to display in the Quantitative Results Table.

### 7.5.14 Change the Display of Chromatograms and Results Tables

Use the [Display] tab in the [Summary (Data) Properties] sub-window to change the horizontal and vertical chromatogram display and table information to display.

**1** **Click the [Display] tab.**

**2** **Set the [Display] tab parameters, and click [OK].**




1 Click [Right Chromatogram] to display the table on the right side of the chromatogram.
2 Change [Arrangement] to change the display aspect ratio of chromatograms and tables.

## 7.6 Report Layout

Functions for editing the positions of report items include position and size adjustment, header/footer setting and the ability to add, move or delete pages.

### 7.6.1 Change the Item Position and Number of Pages

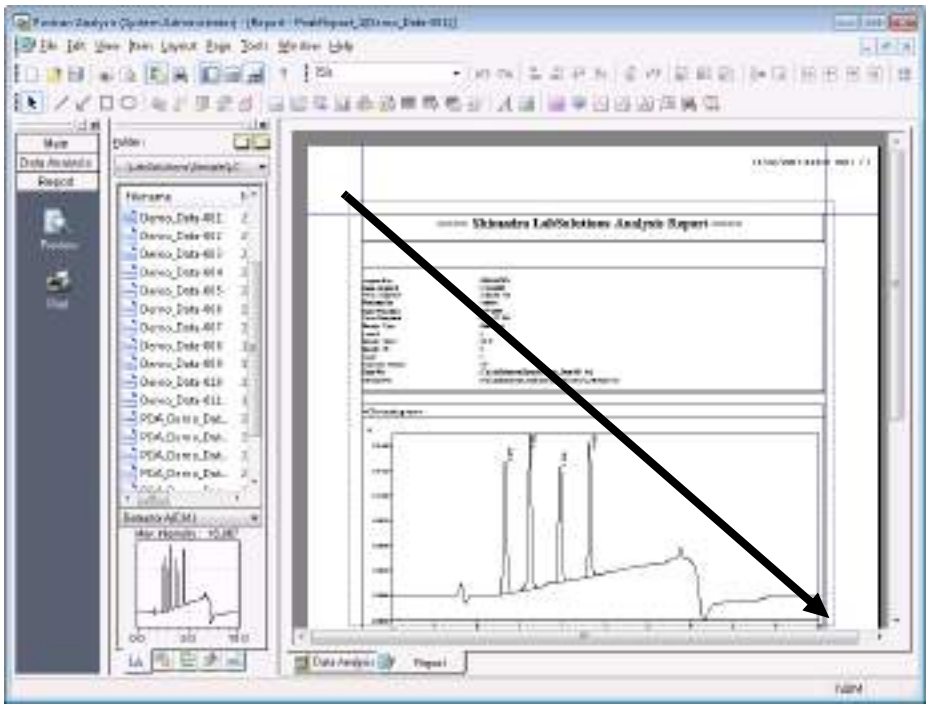
If a report format includes multiple items, the layout icons are enabled in the toolbar so that the items can be repositioned.

Pages can be added to and deleted from the report format.

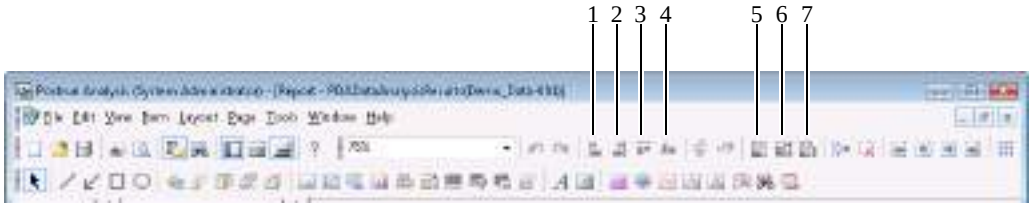
## ■ Re-Position Items

**1** Click (Pointer) on the toolbar.

**2** Drag the point so that it encloses the items to be re-positioned.



**3** Click each of the items on the [Report] toolbar, and adjust the position of items.




| No. | Explanation |
|---|---|
| 1 | Aligns items to the left edge of the left most item. |
| 2 | Aligns items to the right edge of the right most item. |
| 3 | Aligns items to the top edge of the topmost item. |
| 4 | Aligns items to the bottom edge of the bottommost item. |
| 5 | Aligns the width of each item to the longest horizontal item. |
| 6 | Aligns the height of each item to the longest vertical item. |
| 7 | Aligns the width and height of each item to the longest horizontal and vertical item. |

**NOTE**

- Some of the layout icons are disabled if only one item is selected.
- Drag the frame of the report item to resize that item.

### ■ Add or Delete Report Pages


| No. | Explanation |
|---|---|
| 1 | Inserts a page after the currently displayed page. |
| 2 | Deletes the currently displayed page. |
| 3 | Displays the first page. |
| 4 | Displays the previous page. |
| 5 | Displays the next page. |
| 6 | Displays the last page. |

**NOTE**

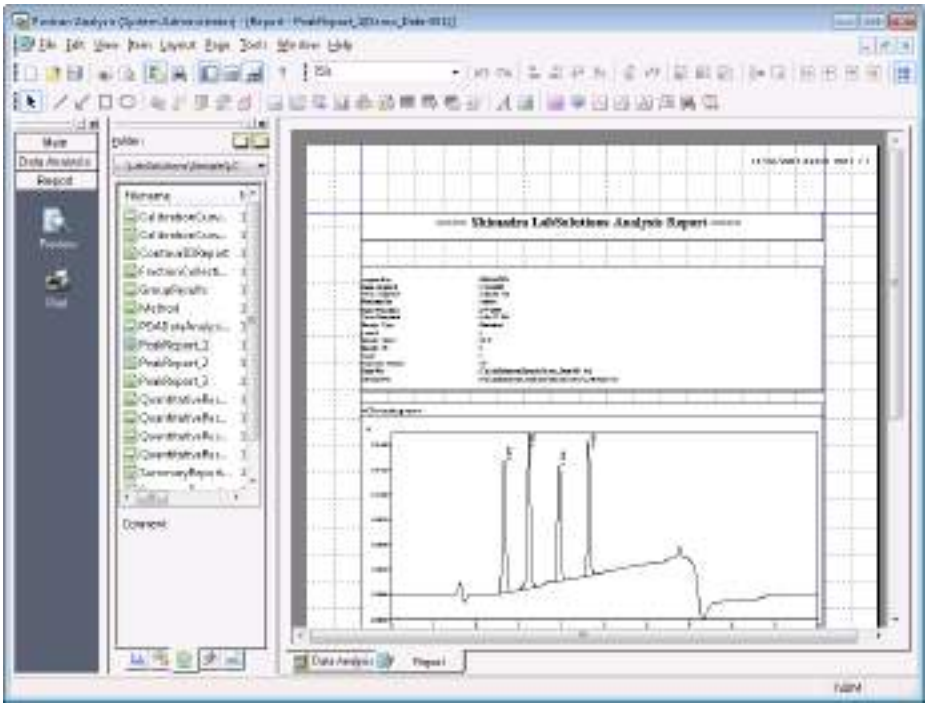
All icons except the [Insert (Page)] icon (1) are disabled if there is only one page.

## 7.6.2 Use the Grid

Use the grid to adjust the positions of report items.

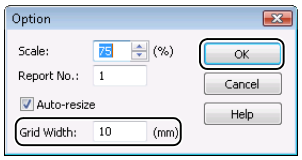
This section describes how to display the grid in the [Report] window.

**1** **Display the report format file on the [Report] window, and click (Toggle Grid) on the toolbar.**



**2** **To adjust the interval of the displayed grid, click [Option] on the [View] menu.**

**3** **Enter [Grid Width], and click [OK].**




The grid is displayed at that interval.

## 7.6.3 Headers and Footers

This section describes how to display information such as, print date, page number in the header or footer of the report format.

**1** **Display the report format file on the [Report] window, and click [Header/Footer] on the [View] menu.**

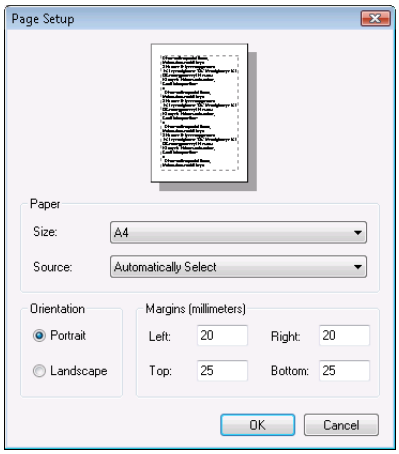
**2** **Select the [Header] or [Footer] tab and select the information to be displayed in the [Left], [Center], and [Right] sections.**

**3** **Click [OK].**

The settings are displayed in the report header or footer.

### 7.6.4 Paper Size and Margin

Click [Page Setup] on the [File] menu in the [Report] window. The [Page Setup] sub-window is displayed. Select the paper size, paper source, orientation (portrait or landscape), and margins of the report.




## 7.7 Other Reports

Exclusive reports can also be output from the following sub-windows.

| Window/Sub-Window | Explanation (Operation Method) |
|---|---|
| Data Acquisition | The contents of the displayed method file are loaded to a system exclusive report format and output. ([Print Method File] on the [File] menu) |
| System Configuration | The current system configuration information is loaded to a system exclusive report format and output. ([Print] button) |
| Realtime Batch<br>Postrun Batch | The contents of the Batch Table are loaded to a system exclusive report format and output. Edit the report format to match specific display items.<br>([Print Batch Table] on the [File] menu) |
| Data Analysis<br>PDA Data Analysis<br>MS Data Analysis<br>Calibration Curve<br>Data Comparison<br>UV Library Editor<br>Quant Browser | The contents of files loaded to each window can be loaded to a system exclusive report format and output. |
| Spectrum Index | The PDA chromatograms and spectra for detected peaks are loaded to a system exclusive report format and output.<br>([Print Spectrum Index] on the [File] menu in the [PDA Data Analysis] window) |
| Spectrum Table | Spectrum information registered to the Spectrum Table is output. |
| UV Library Search Results | The UV library search results are loaded to an exclusive report format and output. Edit the report format to match the settings made in the data processing parameters.<br>([Print] on the [Library Search] menu) |
| MS Library Search Results | The MS library search results are loaded to an exclusive report format and output.<br>([Print] on the [Search Results] of [Report] menu) |
| Audit Trail Log | If the audit trail log is activated, the log contents are output in a fixed format. ([Print] button) |
| Log Browser | Each log displayed in the log browser is output in a fixed format. |
| Show Check Result | Results of the program or raw data check are output in a fixed format. |
| System Check Results | The system check results are output in a fixed format.<br>([Print] button) |

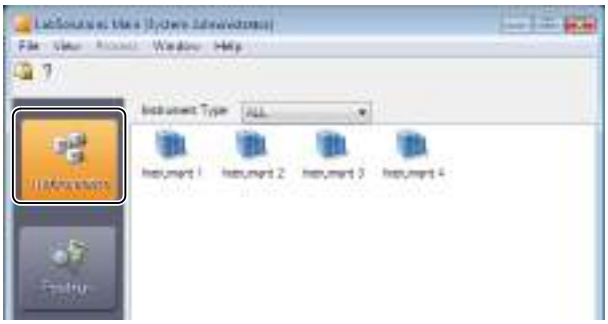
# 8 Tuning

This chapter describes how to perform the tuning process to optimize MS control parameters. Two tuning modes, auto-tuning and manual tuning are described in the chapter.

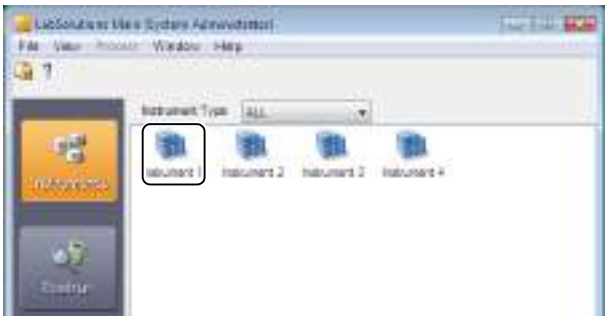
## 8.1 [MS Tuning] Window

### 8.1.1 Open the [Data Acquisition] Window

**1** **Click the**  **icon.**



**2** **Select and double-click the instrument on which data acquisition will be performed.**



The [Realtime Analysis] program opens.

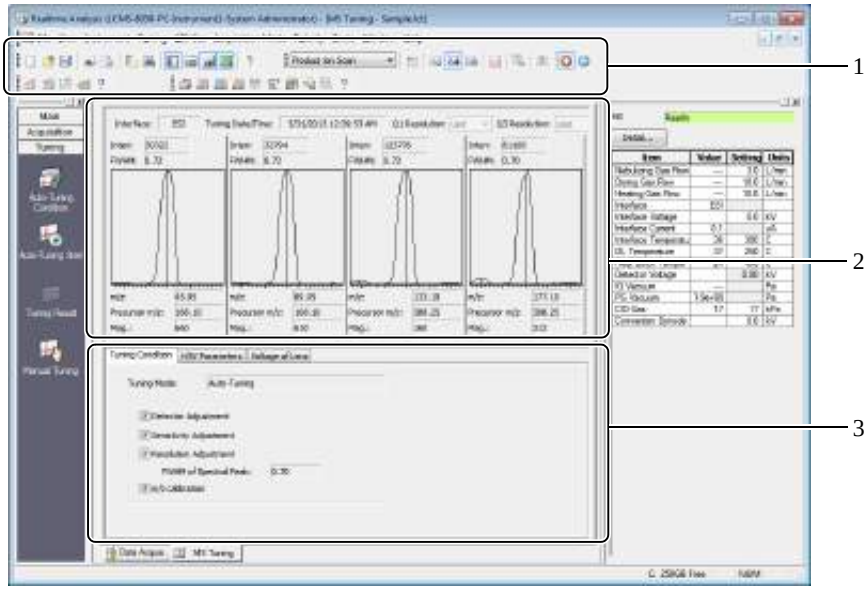
**3** **Click the**  **(Tuning) icon on the [Main] assistant bar.**

**NOTE**

Click Main on the title of the assistant bar if the  (Tuning) icon is not displayed.

## 8.1.2 [MS Tuning] Window Description

This section describes how to view and use the [MS Tuning] window.




| No. | Explanation |
|---|---|
| 1 | Displays the [Standard], [Instrument Control], [LC Control], [PDA Control], [MS Control], and [MS Tuning] toolbars. |
| 2 | Displays the profile spectrum in the auto-tuning mode or manual tuning mode. |
| 3 | Displays the tuning conditions and tuning results. |

# 8.2 Auto-Tuning

Use the auto-tuning mode to optimize various control parameters of the MS instrument according to preset auto-tuning conditions.

**NOTE**

Before auto-tuning, verify the amount of sample in the standard sample bottle.

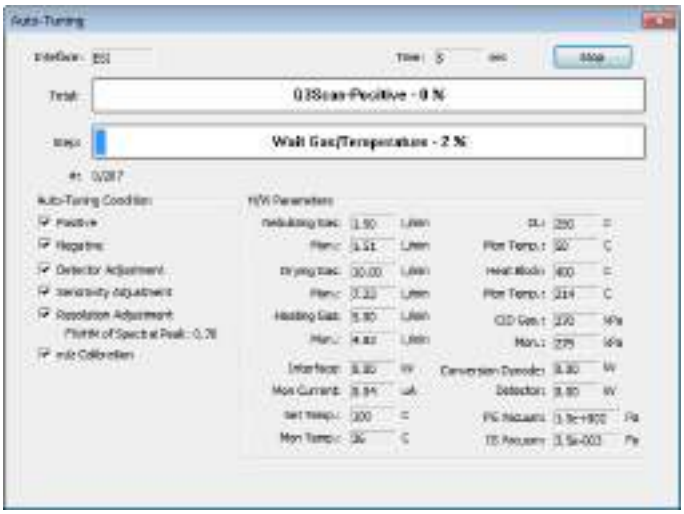
Verify that the standard sample flow path to ensure that it is correctly injected into the MS instrument.

## 8.2.1 Execute Auto-Tuning

**1** **Select [Print Result after Auto Tuning] on the [Tuning] menu to print the results when auto-tuning is complete.**

**2** **Click the (Start Auto Tuning) icon on the [Tuning] assistant bar.**

The [Auto Tuning] sub-window is displayed, and the auto-tuning process is initiated. Check the tuning status in the [Auto Tuning] sub-window.



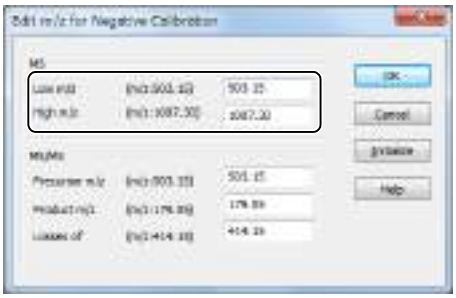
After tuning is complete with no error messages, the standard sample spectrum is acquired using the preset tuning parameters. Then, the spectrum and optimized parameters are displayed in the tuning result mode.

**Reference**

Refer to *"8.2.2 Check Tuning Results" P.281* for details on the tuning result mode.

**NOTE**

- Auto-tuning is an extensive process since it searches for the optimum parameters.
- The most probable cause of auto-tuning errors not related to the MS instrument is when the standard sample is not correctly introduced into the MS instrument.Verify that there is sufficient standard sample and that there are no problems with the flow path.
- Peak sensitivity used for calibration during negative tuning can decrease significantly depending on the type of mobile phase. If this occurs, click [m/z for Negative Calibration] on the [Tuning] menu and edit the *m/z* value.



**3 Click (Save) on the toolbar.**

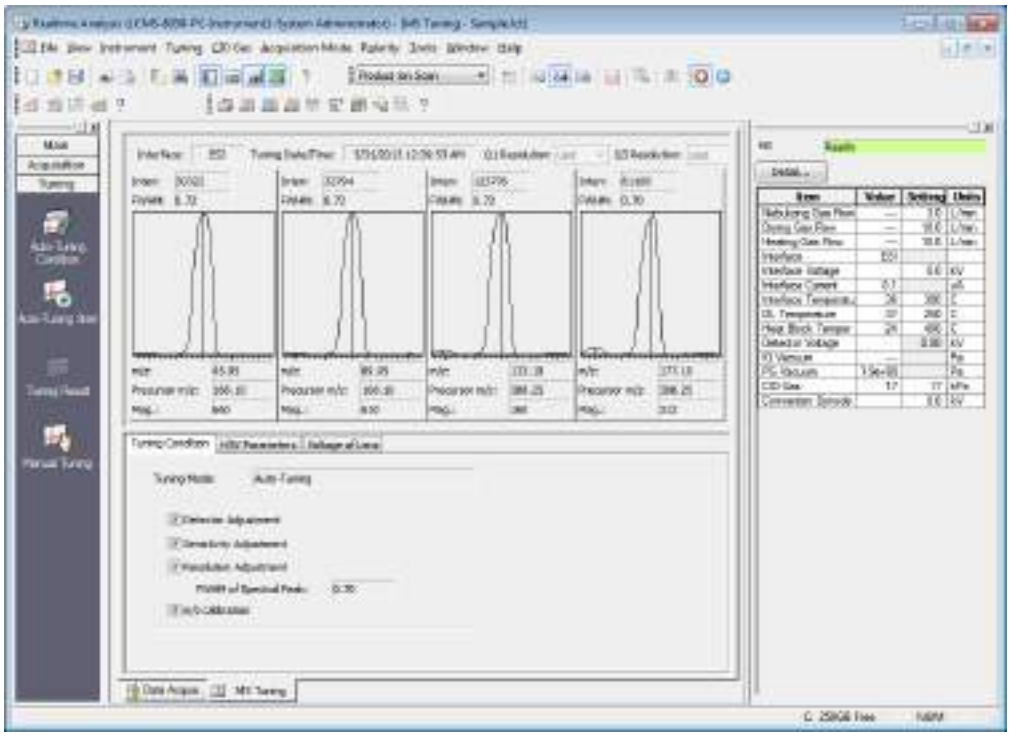
The new control parameters are saved to a tuning file (file extension *.lct).
When the tuning file is saved, a message to confirm whether or not to use this file as default is displayed. Once this file is applied as default, it will be used as the tuning file when any tuning file is not set in single run or realtime batch.

## 8.2.2 Check Tuning Results

Tuning results can be checked on the [Tuning] assistant bar in real time.

**1** **Click the (Result Tuning) icon on the [Tuning] assistant bar.**


Tuning results are displayed in the tuning result mode.
In this mode, the tuning results saved to the currently loaded tuning file are displayed.



**NOTE**

- When the [Tuning] window is opened, the specified default tuning file is automatically loaded.
- Unless otherwise specified, the tuning file loaded here is used in system checks or in data acquisition.

### 8.2.3 Repeat Auto-Tuning

If there is a problem with the tuning results, auto-tuning is only repeated for the required items such as resolution adjustment, sensitivity adjustment or mass calibration.

**1** **Click the (Auto Tuning Condition) icon on the [Tuning] assistant bar.**


**2** **Select the required items, and click [OK].**


Auto-tuning is executed only for the selected items.
Click [Only Positive Tuning] to perform tuning only on items with a positive polarity.
A small [FWHM] value improves resolution but lowers sensitivity.

## 8.3 Manual Tuning

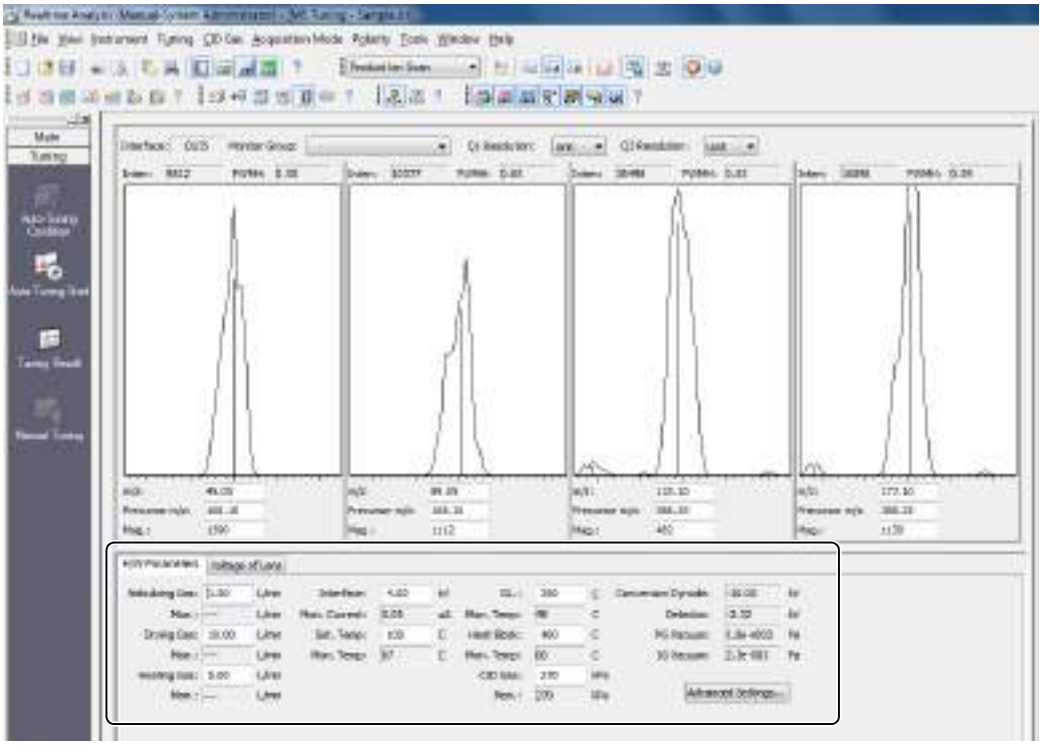
Use the manual tuning mode to correct the control parameters that were determined by auto-tuning and verify that the tuning results are satisfactory.

**1** **Click the (Manual Tuning) icon on the [Tuning] assistant bar.**


The mode changes to the manual tuning mode, and acquired data is loaded in real time.
Each of the MS control parameters can be edited in the manual tuning mode.

**2** **Check the conditions of the standard sample ion peak.**
**Click the respective tab, and directly edit the MS control parameters.**

**NOTE**
Select [m/z Calibration] from the [Tuning] menu to manually calibrate the mass axis.



**3** **Click (Standard Sample) on the toolbar, and introduce the tuning sample into the flow path.**

The MS spectrum is displayed in each cell. New parameter settings are sent to the MS instrument in real time.
Fine-adjust the MS control parameters while checking the spectrum.

**NOTE**

- Do not click (Standard Sample) if the tuning standard is not being injected from the standard sample bottle. Use the solvent delivery unit to inject the sample like a regular sample, or directly introduce the sample to the mass spectrometer by infusion acquisition.
- Auto-tuning is normally sufficient and specialist knowledge of MS instruments is required to change the control parameters with manual tuning.
- Quantitative results are influenced if the standard sample data used for the calibration curve and the unknown sample data are acquired under different tuning conditions.

# 9 Method Optimization

Method optimization refers to a function that sets the voltage value in instrument parameters for an SIM or MRM event to an optimal value or adjusts the *m/z* values for precursor and product ions.

If the *m/z* values for product ions are not known, an automatic search function is available as well. Optimization results are saved in a method file and can be confirmed at any time.

This chapter describes the basic process flow for optimizing an MRM event.

## 9.1 Process Flow from Method Optimization to Quantitation

**[Data Acquisition] window**

Step 1 Use flow injection analysis (FIA) to optimize MRM events.

**To automatically search for precursor ions**

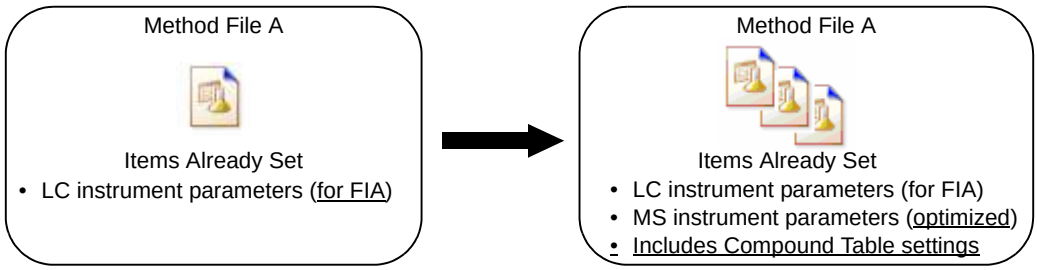
**Reference**

*"9.2 Optimize Methods by Searching Precursor Ions and Product Ions" P.287*

**To automatically search for product ions**

**Reference**

*"9.3 Optimize Methods by Specifying Only m/z Values for Precursor Ions" P.293*




**Example of LC instrument parameters for the flow injection analysis**

Pump Flow: 0.2 mL/min

[LC Stop Time] on the [Data Acquisition] tab:0.5 min

[Stop] command on the [LC Time Prog.] tab: 0.5 min

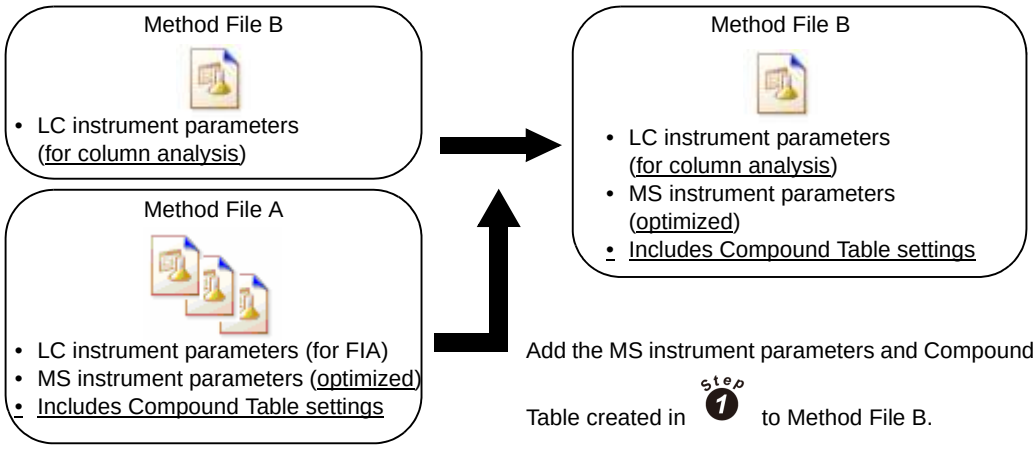
No Column

### Continuation of [Data Acquisition] window

Step 2 Perform column analysis on a standard sample to investigate compound retention times.

**Reference**

*"9.4 Check Compound Retention Times" P.297*

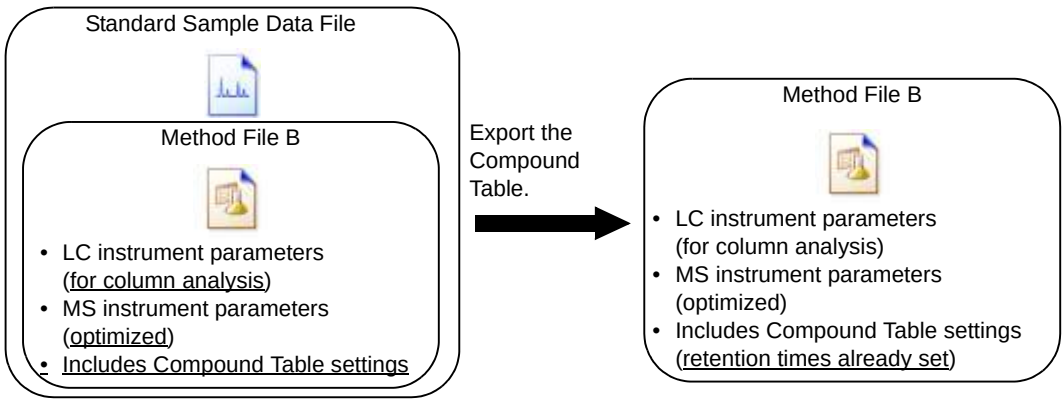



### [MS Data Analysis] window

Step 3 Set retention times in the Compound Table by confirming peaks in the standard sample measurement data.

**Reference**

*"9.5 Set Retention Times in the Compound Table" P.300*

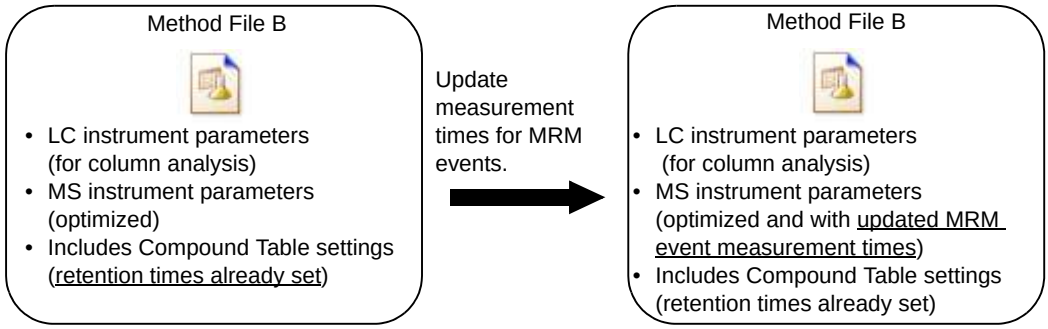


**[Data Acquisition] window**

Step 4 Based on retention times in the Compound Table, update the measurement times for MRM events set in instrument parameters.

**Reference**

*"9.6 Update Measurement Times in MRM Events" P.305*




**[Realtime Batch] and [Quant Browser] Windows**

Step 5 Perform realtime batch on standard and unknown samples and perform quantitative processing.

**Reference**

*"9.7 Create a Calibration Curve and Perform Quantitative Calculations" P.307*



# 9.2 Optimize Methods by Searching Precursor Ions and Product Ions

Precursor Ions are determined based on the specified Precursor Ion auto selection conditions and Product Ions based on the specified Product Ion auto selection conditions. Then it optimizes the method.

## 9.2.1 Prepare the Sample

**1 Remove the column to allow flow injection analysis.**

**2 Place the samples for optimization on the autosampler.**

## 9.2.2 Open the [Data Acquisition] Window

**1** **Start up the [Realtime Analysis] program from the [LabSolutions Main] window to open the [Data Acquisition] window.**

**Reference**

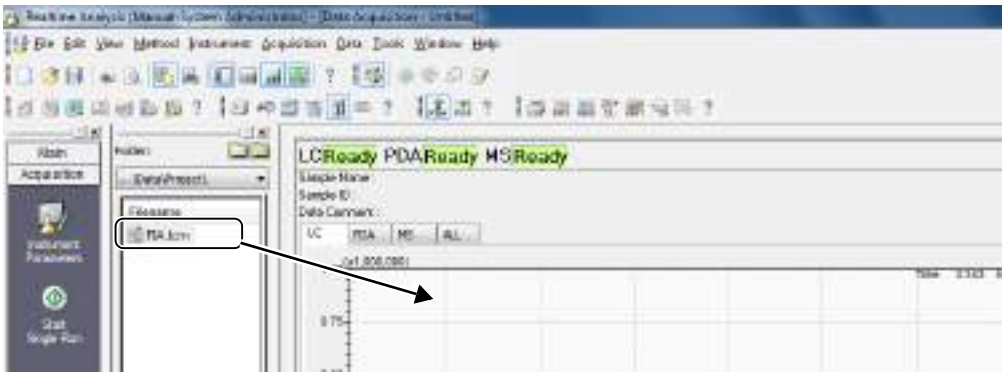
For details on operations, see *"2.1.1 Open the [Data Acquisition] Window" P.9*.

**2** **Select a method file set with the LC and MS instrument parameters.**

**NOTE**

Set LC instrument parameters to flow injection analysis.

1 Drag-and-drop the method file onto the [Data Acquisition] window from the [Data Explorer] sub-window.




**Reference**

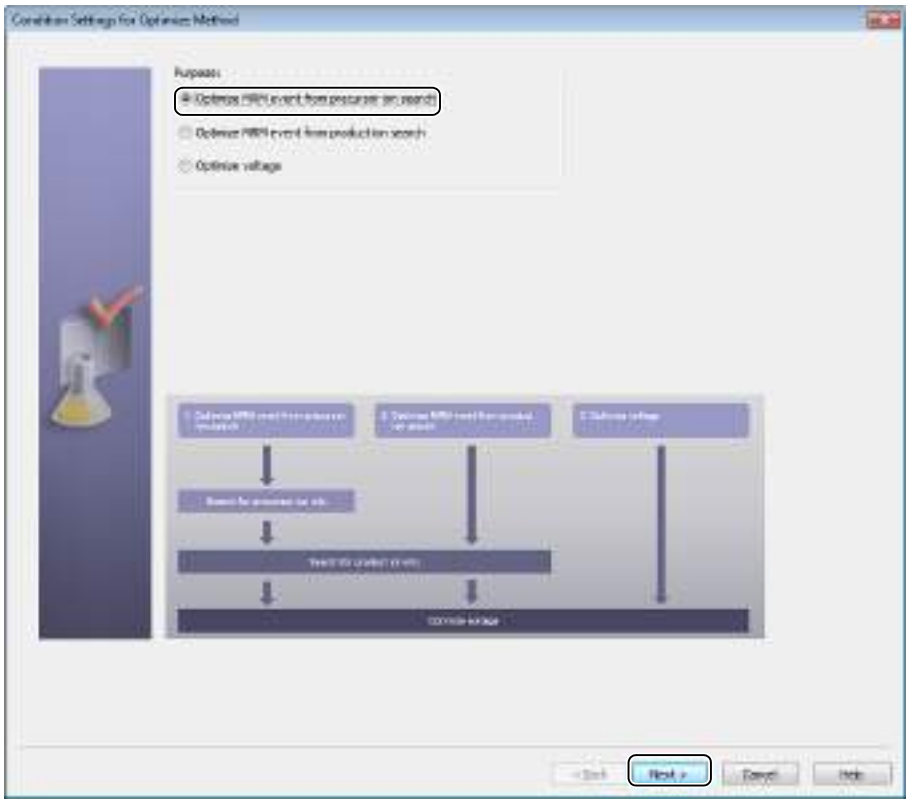
For details on instrument parameter setting, see *"2.2.2 Set the LC Instrument Parameters" P.12*.

## 9.2.3 Optimize Method

**1** **Click the**  **(Optimization for Method) icon on the [Acquisition] assistant bar.**

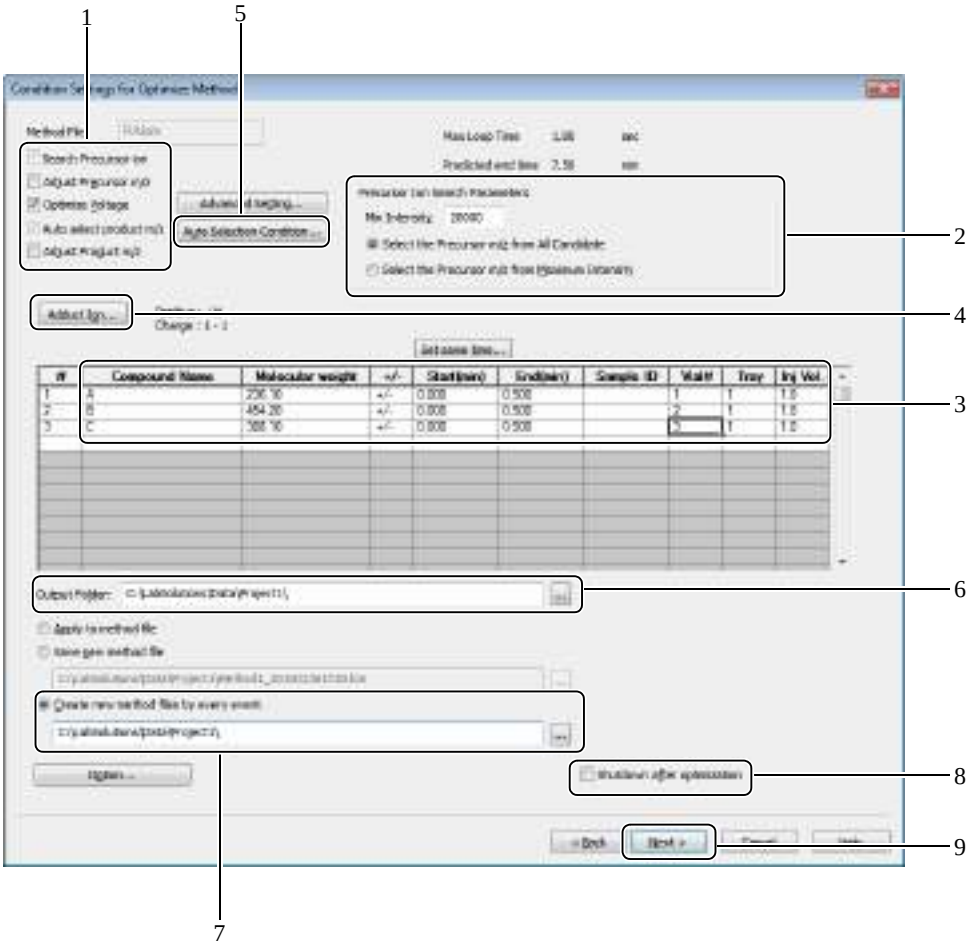
The [Condition Settings for Optimize Method] sub-window is displayed.

**2** **Click [Optimize MRM event from precursor ion search], and click [Next].**



The [Condition Settings for Optimize Method] sub-window is displayed.

## 3 Set the optimization conditions, and click [Next].




Optimize each event by measuring the sample for each item selected in area 1.

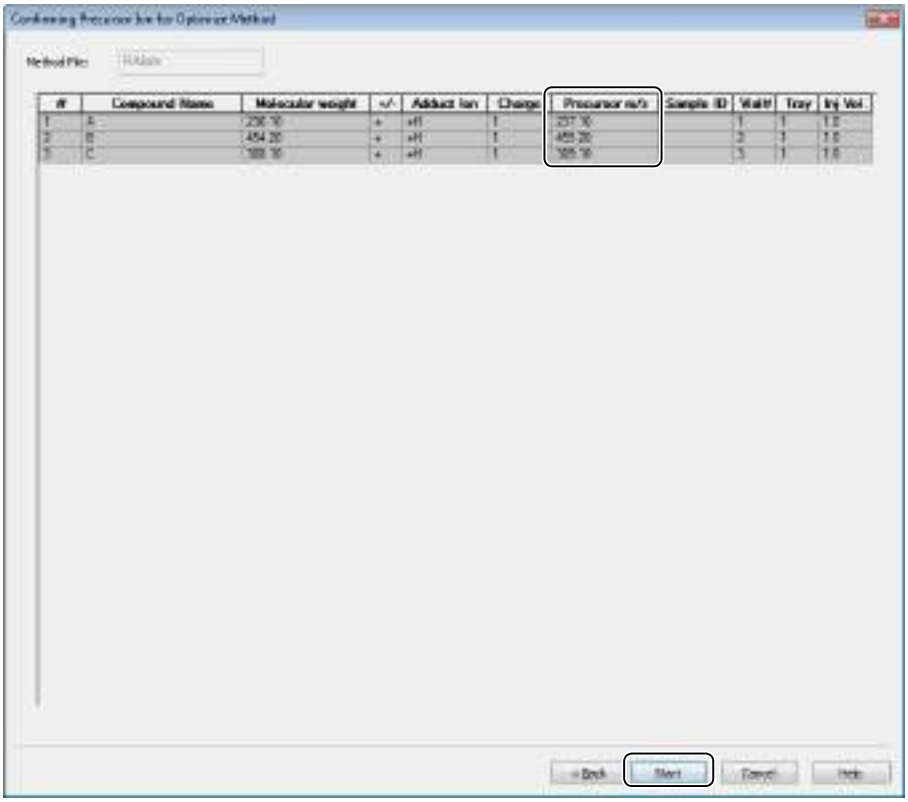
| No. | Description |
|---|---|
| 1 | At [Search Precursor ion], data acquisition is executed once for automatically searching the *m/z* of the Precursor Ions. Precursor ion *m/z* values are calculated by the combination of molecular weight set at 3 and adduct ions, polarities, and charges set at 4. When the peaks of precursor ion are observed, the *m/z* values (molecular weight + adduct) are used. Also, the precursor ion *m/z* to use are not actual measured values when observing peaks but theoretical values by calculating.<br>When [Adjust Precursor m/z] is selected, the *m/z* value with the highest peak intensity within the -0.5 to +0.5 u range is determined for precursor ion *m/z*.<br>When [Optimize Voltage] is selected, the items selected for optimization in the [Optimize voltage settings] sub-window, which is displayed by clicking [Advanced Settings], are optimized.<br>When [Adjust Product m/z] is selected, the *m/z* value with the highest peak intensity within the -0.5 to +0.5 u range is determined for product ion *m/z* identified by automatic searching. (Normally, these parameters do not need to be set.) |
| 2 | Sets the minimum intensity value of the ion selected as Precursor Ion.<br>If [Select the Precursor m/z from All Candidate] is selected, the Precursor Ion is determined from all Precursor Ion candidates in search results.<br>If [Select the Precursor m/z from Maximum Intensity] is selected, the Precursor Ion with the maximum intensity is determined from all Precursor Ion candidates in search results. |

| No. | Description |
|---|---|
| 3 | Set the [Compound Name], [Molecular weight], and [+/-] settings for events.<br>Set the measurement times at [Start (min)] and [End (min)].<br>Enter the vial number, tray, and injection volume for samples used for optimization.<br>It indicates information about samples prepared in *"9.3.1 Prepare the Sample"*.<br><br>**NOTE**<br>• If the LC end time value is greater than the specified end time value, the LC end time is applied.<br>• Since the analysis is performed without column, please set a short analysis time.<br>• Parameters set here are applied to the [MS] tab in [Instrument Parameters View]. |
| 4 | Click [Adduct Ion] to set the information of the adduct ions to add or detach.<br>[Adduct Ion Settings] sub-window is displayed.<br><br>  <br>Sets the formula or molecular weight and charges of the adduct ion, and then click [OK] to return to the previous sub-window. |
| 5 | Click [Auto Selection Condition] to set criteria for selecting product ions.<br>The [Auto Selection Condition Settings] sub-window is displayed.<br><br>  <br>Set product ion conditions, and then click [OK] to return to the previous sub-window. |
| 6 | A subfolder is created under the folder specified here. The name of the subfolder is determined by the date and time. The files automatically created during the optimization are output in this folder.<br><br>**NOTE**<br>The default is the project folder. |
| 7 | Select [Create new method files by every event] to create a method file for each compound, and specify the folder to save the method file.<br>The method files are saved using the method file name prefixed with a compound name and event number.<br>Example: "A_1_FIA.lcm" |
| 8 | When [Shutdown after optimization] is selected, realtime batch is executed after optimization is finished.<br>When performing shutdown after optimization, the method file currently opened is closed. |
| 9 | Click [Next].<br>The [Confirming Precursor Ion for Optimize Method] sub-window. |

**NOTE**

If optimization results for each compound are saved in separate method files, methods can be created later by adding only the compounds required.
For details, see *"9.4.2 Create a Method File for Column Analysis" P.297*.

## 4 Confirm the precursor ion m/z values, and click [Start].

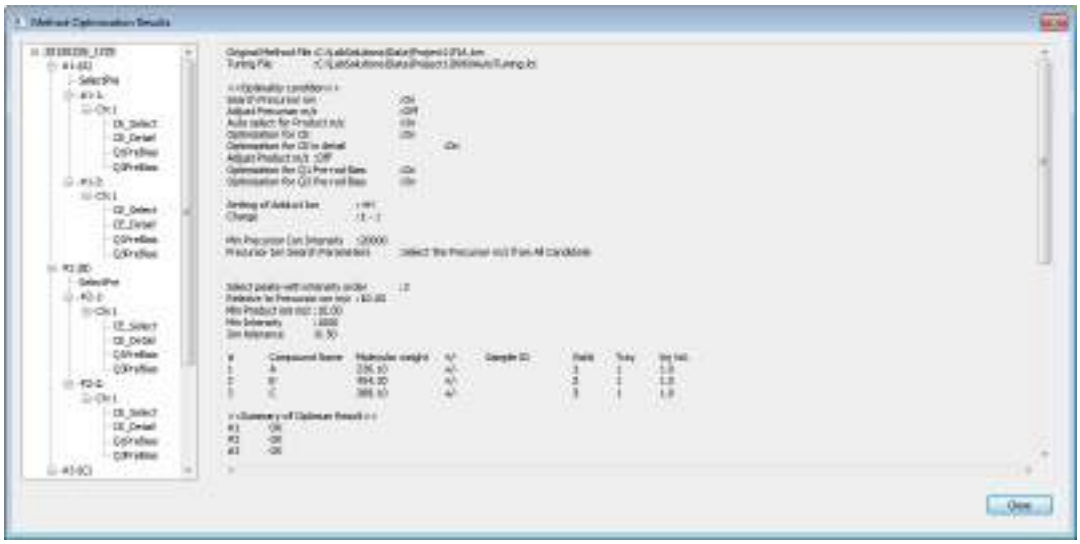


**NOTE**

The [Proceeding for Optimize method] sub-window is displayed during optimization. Clicking [Stop] stops method optimization.

### 9.2.4 Display Optimization Results

After optimization is finished, click [Detail] in the [Proceeding for Optimize method] sub-window to display the [Method Optimization Results] sub-window.



**NOTE**

- The displayed items vary according to the MS detector model.
- After the [Proceeding for Optimize method] sub-window is closed, optimization results can be displayed by clicking [Optimization Result] on the [Method] menu in the [Data Acquisition] window.
- The data files output during the optimization are saved in the folder set at 6. To check detailed results, open the target data file in the [MS Data Analysis] window.

## 9.3 Optimize Methods by Specifying Only *m/z* Values for Precursor Ions



Use this procedure to optimize methods when only the *m/z* values for precursor ions are known and product ions are unknown. This searches for product ions according to the set automatic selection conditions.

### 9.3.1 Prepare the Sample

**Reference**

See *"9.2.1 Prepare the Sample" P.287*.

### 9.3.2 Open the [Data Acquisition] Window

**Reference**

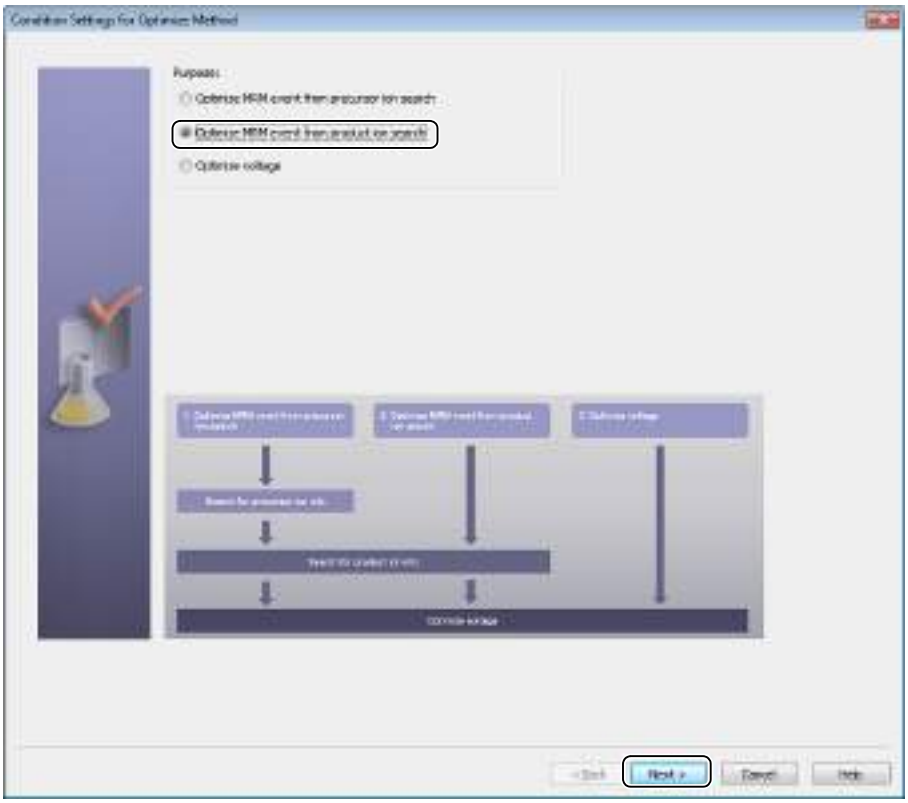
See *"9.2.2 Open the [Data Acquisition] Window" P.288*.

## 9.3.3 Optimize Method

**1** **Click the  (Optimization for Method) icon on the [Acquisition] assistant bar.**

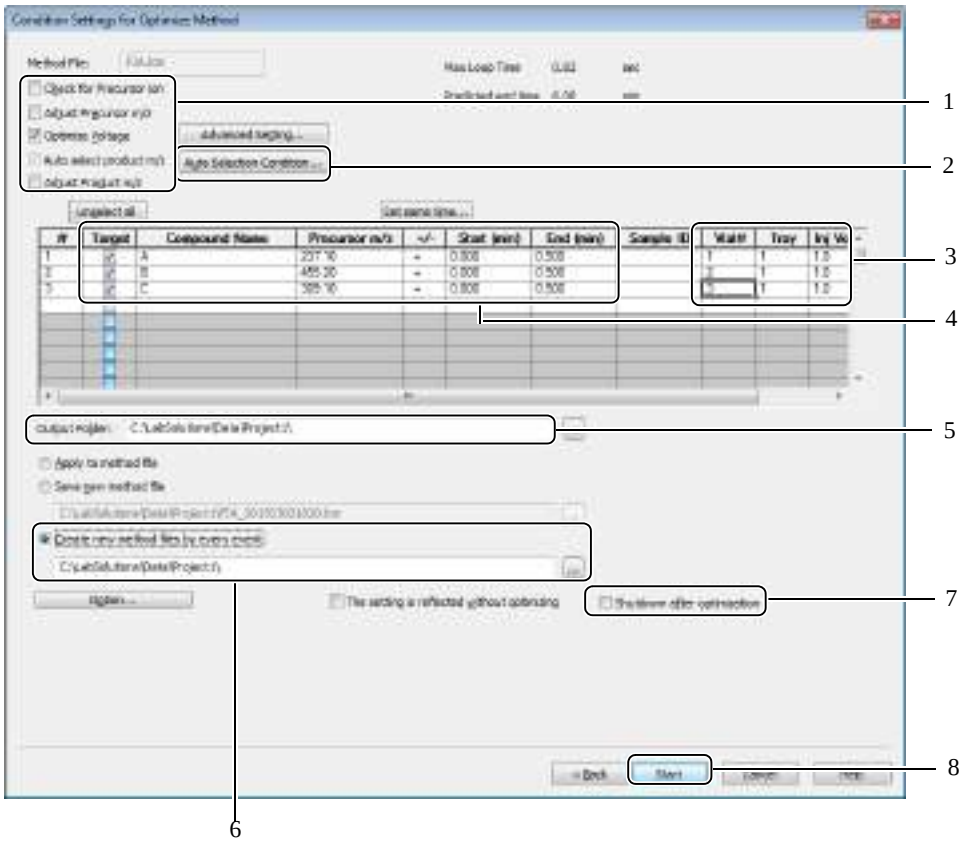

The [Condition Settings for Optimize Method] sub-window is displayed.

**2** **Click [Optimize MRM event from product ion search], and click [Next].**




The [Condition Settings for Optimize Method] sub-window is displayed.

## 3 Set the optimization conditions, and click [Start].



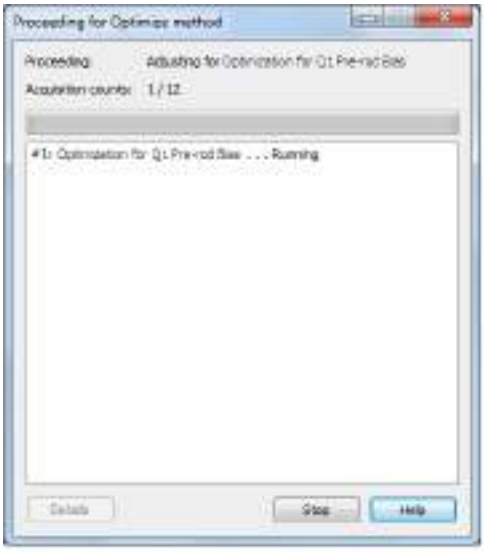

Optimize each event by measuring the sample for each item selected in area 1.

| No. | Description |
|---|---|
| 1 | When [Check for Precursor ion] is selected, data acquisition is executed once to check whether or not precursor ions exist.<br>When [Adjust Precursor m/z] is selected, the *m/z* value with the highest peak intensity within the -0.5 to +0.5 u range is determined for precursor ion *m/z*.<br>When [Optimize Voltage] is selected, the items selected for optimization in the [Optimize voltage settings] sub-window, which is displayed by clicking [Advanced Settings], are optimized.<br>When [Adjust Product m/z] is selected, the *m/z* value with the highest peak intensity within the -0.5 to +0.5 u range is determined for product ion *m/z* identified by automatic searching. (Normally, these parameters do not need to be set.) |
| 2 | Click [Auto Selection Condition] to set criteria for selecting product ions.<br>The [Auto Selection Condition Settings] sub-window is displayed.<br>  <br>Set product ion conditions, and then click [OK] to return to the previous sub-window. |
| 3 | Enter the vial number, tray, and injection volume for samples used for optimization.<br>It indicates information about samples prepared in *"9.3.1 Prepare the Sample"*. |

| No. | Description |
|---|---|
| 4 | Set the [Compound Name], [Precursor m/z], and [+/-] settings for events.<br>Set the measurement times at [Start (min)] and [End (min)].<br><br>**NOTE**<br>• If the LC end time value is greater than the specified end time value, the LC end time is applied.<br>• Since the analysis is performed without column, please set a short analysis time.<br>• Parameters set here are applied to the [MS] tab in [Instrument Parameters View]. |
| 5 | A subfolder is created under the folder specified here. The name of the subfolder is determined by the date and time. The files automatically created during the optimization are output in this folder.<br><br>**NOTE**<br>The default is the project folder. |
| 6 | Select [Create new method files by every event] to create a method file for each compound, and specify the folder to save the method file.<br>The method files are saved using the method file name prefixed with a compound name and event number.<br>Example: "A_1_FIA.lcm" |
| 7 | When [Shutdown after optimization] is selected, realtime batch is executed after optimization is finished.<br>When performing shutdown after optimization, the method file currently opened is closed. |
| 8 | Check [Predicted end time], and click [Start]. |

**NOTE**

- If optimization results for each compound are saved in separate method files, methods can be created later by adding only the compounds required.
  For details, see *"9.4.2 Create a Method File for Column Analysis" P.297*.
- The [Proceeding for Optimize method] sub-window is displayed during optimization. Clicking [Stop] stops method optimization.




## 9.3.4 Display Optimization Results

### Reference

See *"9.2.4 Display Optimization Results" P.293*.

# 9.4 Check Compound Retention Times

Perform single run on a standard sample to investigate compound retention times.

## 9.4.1 Prepare for Data Acquisition

**1** **Attach the column.**

**2** **Place the standard sample on the autosampler.**

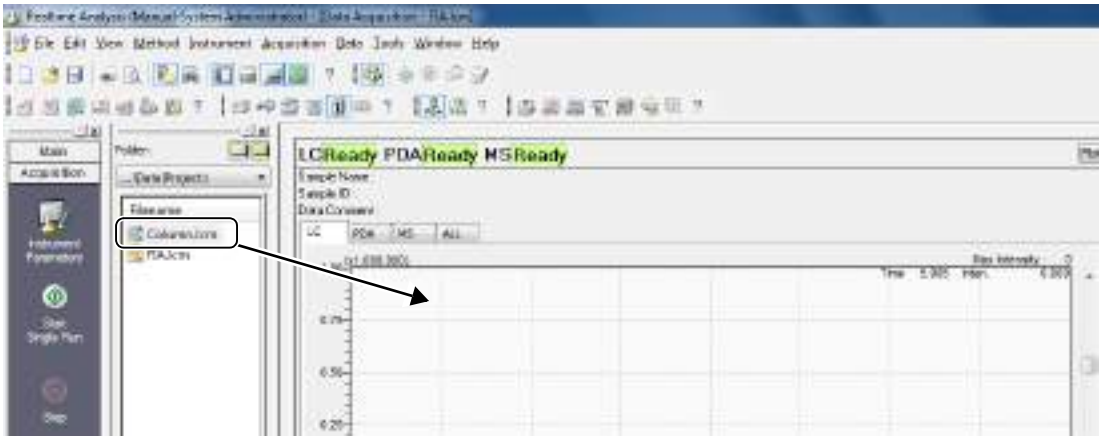
## 9.4.2 Create a Method File for Column Analysis

Add the MRM events set in multiple method files to the Event Table in the method file for column analysis.

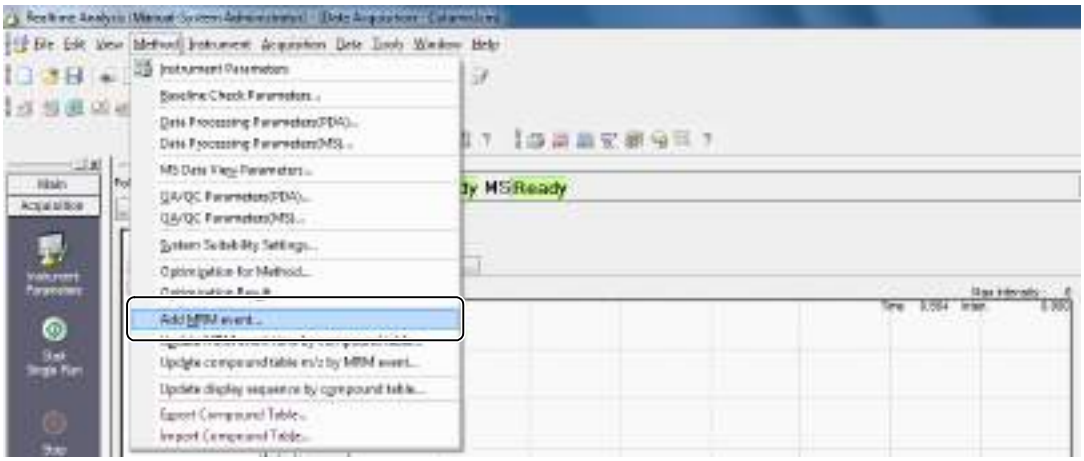
**1** **Select a method file set with the LC and MS instrument parameters.**

**NOTE**
Set LC instrument parameters to column analysis settings.

**2** **Drag-and-drop the source method files onto the [Data Acquisition] window from the [Data Explorer] sub-window.**

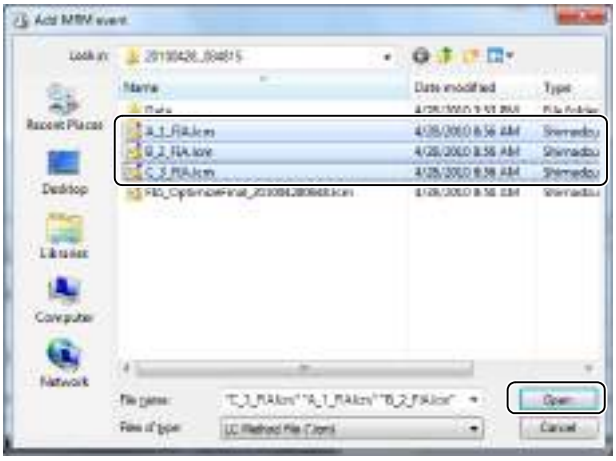


**3** **Click [Add MRM event] on the [Method] menu.**



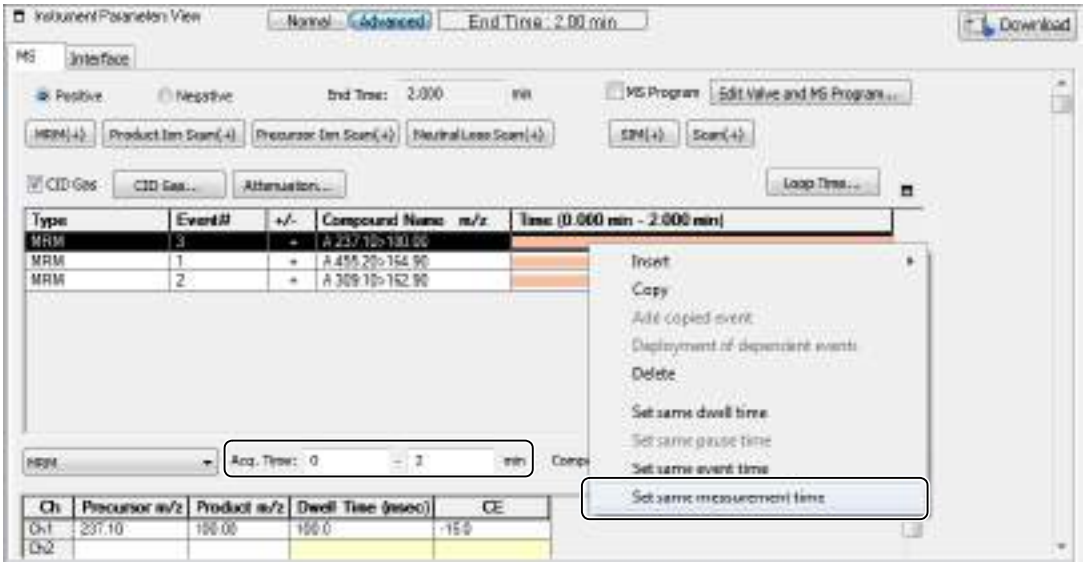

The [Add MRM event] sub-window is displayed.

**4** **Select the method file(s) containing the MRM event settings to add, and click [Open].**

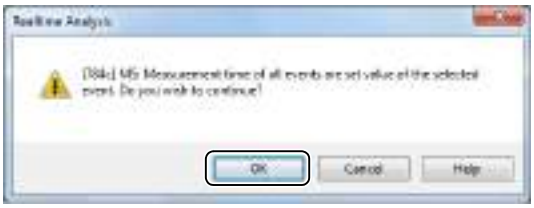



Only the MRM events for the selected method files are added to the end of the Event Table.

**5** **Select one of the events in MS instrument parameters, set the measurement time, and click [Set Same Measurement Time] on the right-click menu.**

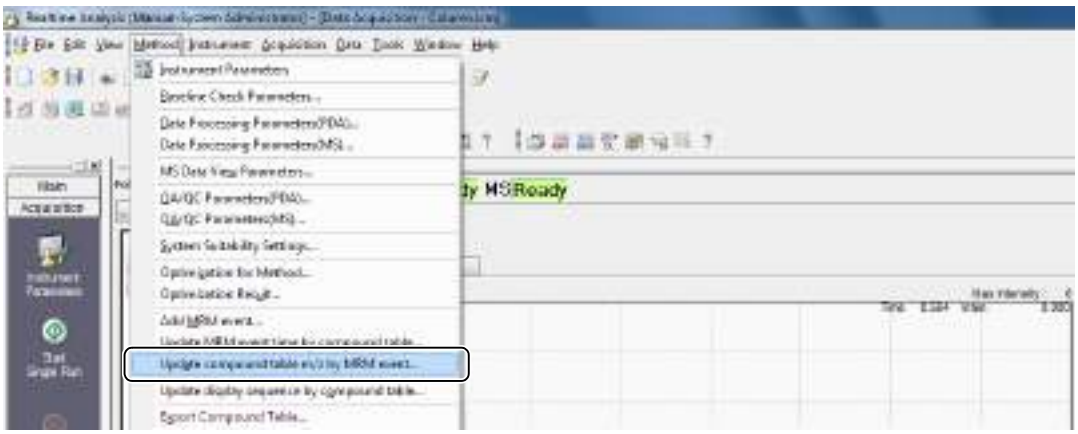



**6** **When the confirmation message is displayed, click [OK].**




This results in the same measurement time for all events.

**7** **Click [Update compound table m/z by MRM event] on the [Method] menu.**




The Compound Table parameters are updated based on the Event Table.

**NOTE**

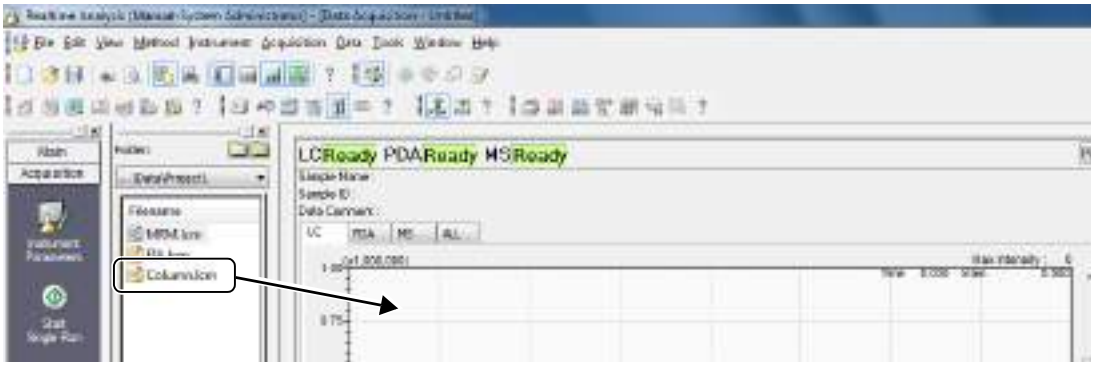
Even if events are added or deleted in the Event Table on the [MS] tab in [Instrument Parameters View], Compound Table parameters are not automatically updated.

**8** **Save the changes in the method file.**

1 Click [Save Method File As] on the [File] menu.
2 Enter the file name in the [Save Method File As] sub-window, and click [Save].
The results of adding the MRM events are saved in the method file.

### 9.4.3 Execute Single Run

**1** **Drag-and-drop the method file for MRM acquisition onto the [Data Acquisition] window from the [Data Explorer] sub-window.**




**2** **Click the**  **(Start Single Run) icon on the [Acquisition] assistant bar.**

**3** **Set the data acquisition settings, and click [OK].**
For details on operations, see *"2.5.1 Execute Single Run" P.36*.

## 9.5 Set Retention Times in the Compound Table

Set the retention times in the Compound Table in the method file used for MRM acquisition while confirming the compound peaks in the data file acquired in *"9.4 Check Compound Retention Times" P.297*.

### 9.5.1 Open the [MS Data Analysis] Window

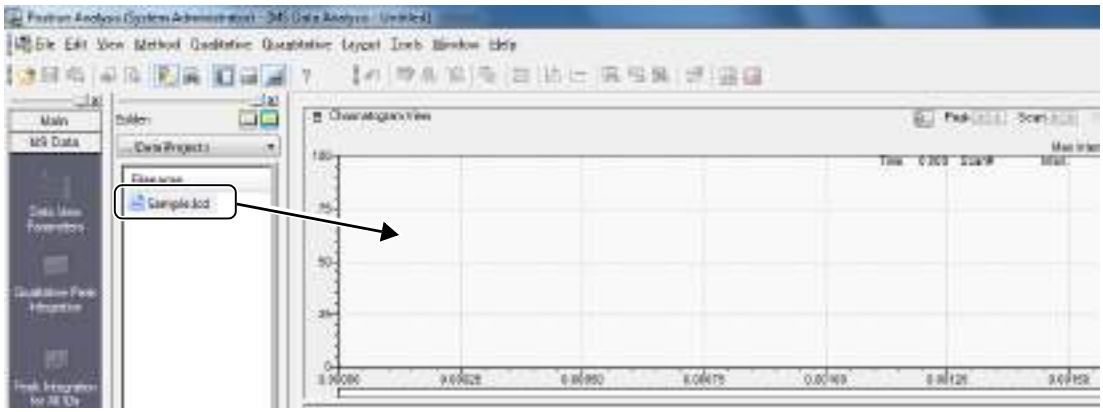
**1** **Click the**  **(Data Analysis) icon on the [Acquisition] assistant bar to open the [MS Data Analysis] window.**

**Reference**
For details on how to use the [MS Data Analysis] window, see *"6.1.2 [MS Data Analysis] Window Description" P.177*.

The [MS Data Analysis] window is displayed.

## 9.5.2 Load Data Files

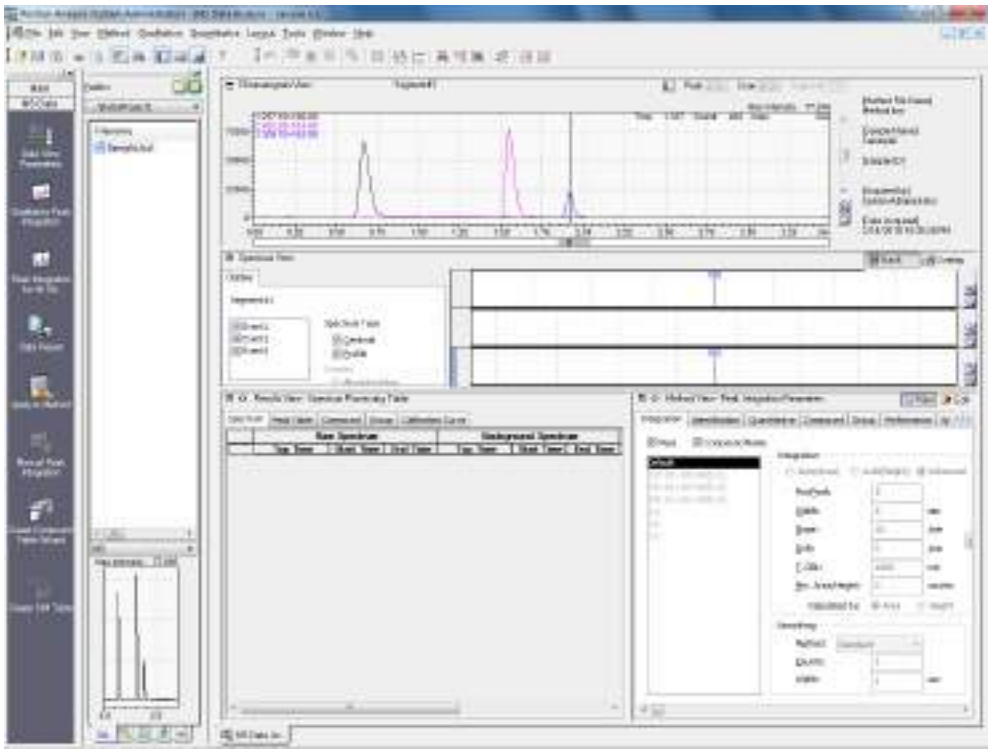
**1** **Drag-and-drop the data file acquired in *"9.4 Check Compound Retention Times"* onto the [MS Data Analysis] window from the [Data Explorer] sub-window.**



The content of the data file is displayed in the [MS Data Analysis] window.

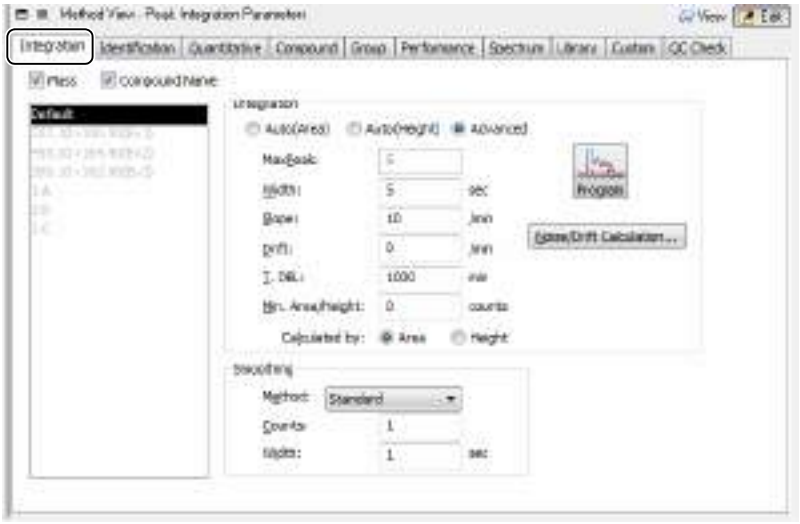
## 9.5.3 Set Retention Times in the Compound Table

**1** **Click <> (Wide Size) in [Method View].**

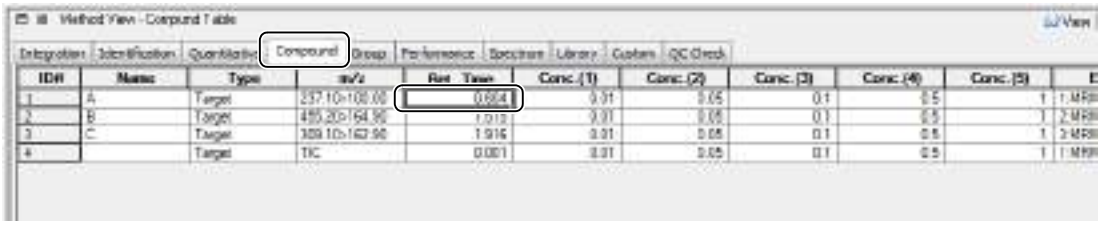


**2** **Click Edit (Edit Mode) in [Method View].**

**3** **Click the [Integration] tab and set each parameter so that the peaks for target compounds can be detected.**

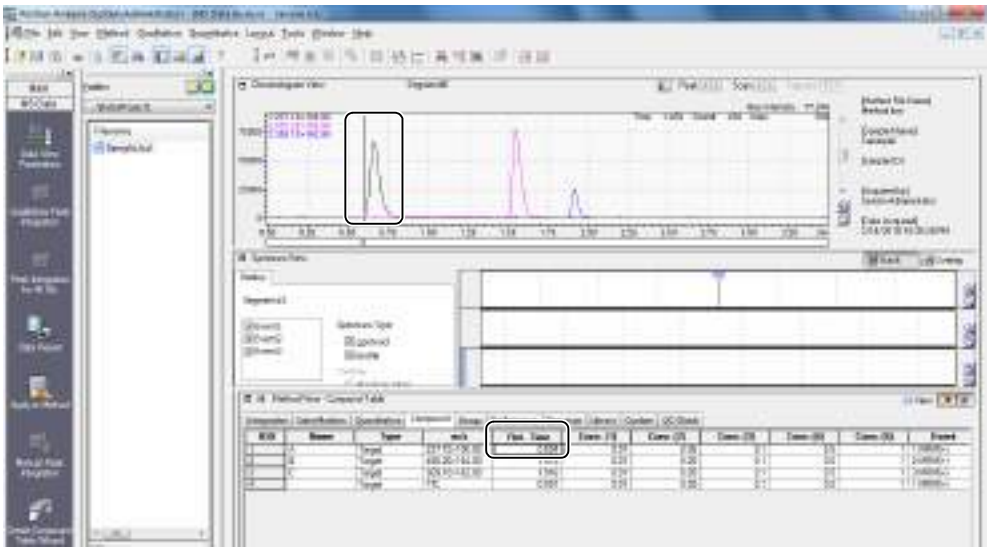


**4** **Click the [Compound] tab, and click the [Ret. Time] cell in the Compound Table.**



**5** **Display a mass chromatogram in [Chromatogram View], and double-click near the peak tops.**

This sets the retention time of the double-clicked position in the [Ret. Time] cell on the [Compound] tab.



**6** **Set the retention times for other compounds as well by repeating steps 4 and 5.**

**7** **Click View (View Mode) in [Method View].**

This applies the newly edited details.

**NOTE**

When the [Peak integration for all IDs will be performed. Continue?] message is displayed, click [Yes].

**8** **Click the (Peak Integration for All IDs) icon on the [MS Data] assistant bar.**


The chromatograms of all IDs on the [Compound] tab in [Method View] undergo quantitative processing (peak integration, identification, and quantitative processing).

**9** **Click (Normal Size).**

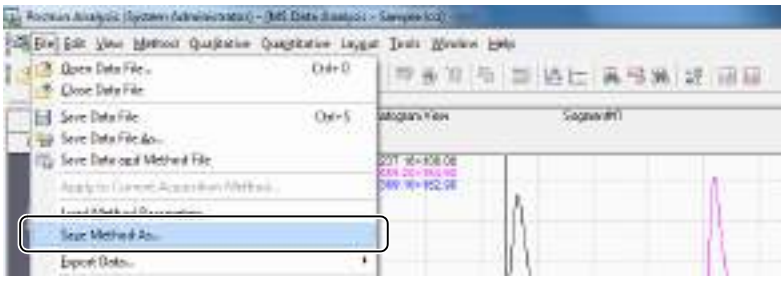
**10** **Click the [Compound] tab in [Result View] and confirm the quantitative calculation results.**

**NOTE**

If no peaks could be detected, change the peak integration parameters on the [Integration] tab in [Method View] and perform quantitative processing again.

## 9.5.4 Save (Export) the Compound Table to a Method File

**1** **Click [Save Method As] on the [File] menu.**



**2** **Enter the name of the MRM acquisition method file in the [Save Method As] sub-window, and click [Save].**

**NOTE**

Data files contain information about method files, batch files, and report format files. The [MS Data Analysis] window allows editing methods in data files and exporting the results. For details on file formats, refer to "System Users Guide".

**3** **Select [Data Processing Parameters] at [MS Data Processing] in the [Select Method Parameters] sub-window, and click [OK].**

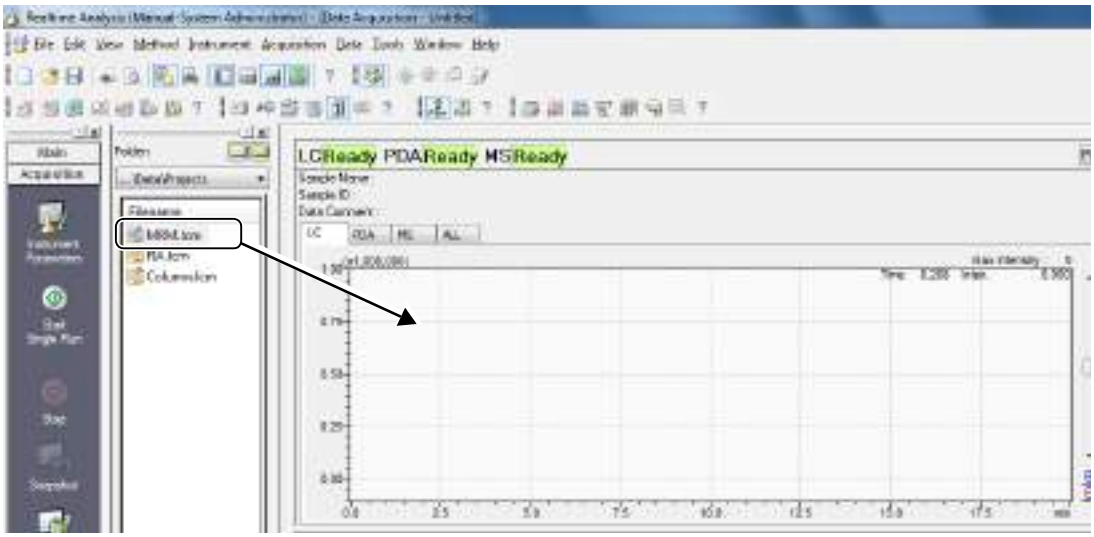
The Compound Table is exported to the method file.

# 9.6 Update Measurement Times in MRM Events

Update MRM event measurement times for MS instrument parameters based on the retention times in the Compound Table set in *"9.5 Set Retention Times in the Compound Table"*.

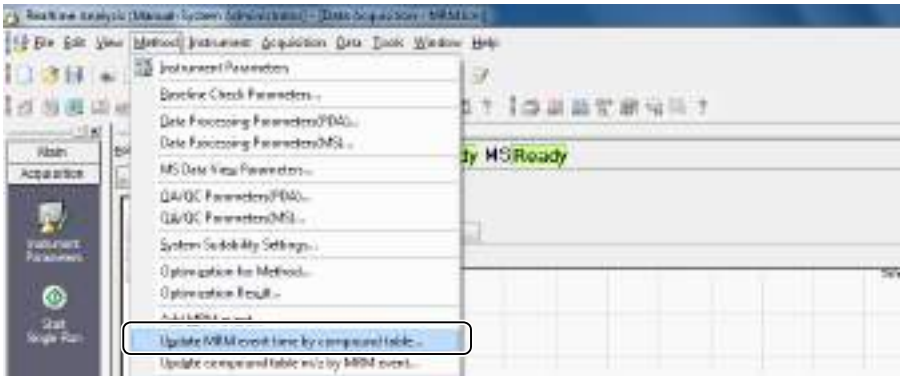
## 9.6.1 Open the [Data Acquisition] Window

**1** **Drag-and-drop the method file for MRM acquisition onto the [Data Acquisition] window from the [Data Explorer] sub-window.**




## 9.6.2 Update Measurement Times in MRM Events

**1** **Click [Update MRM event time by Compound] on the [Method] menu.**

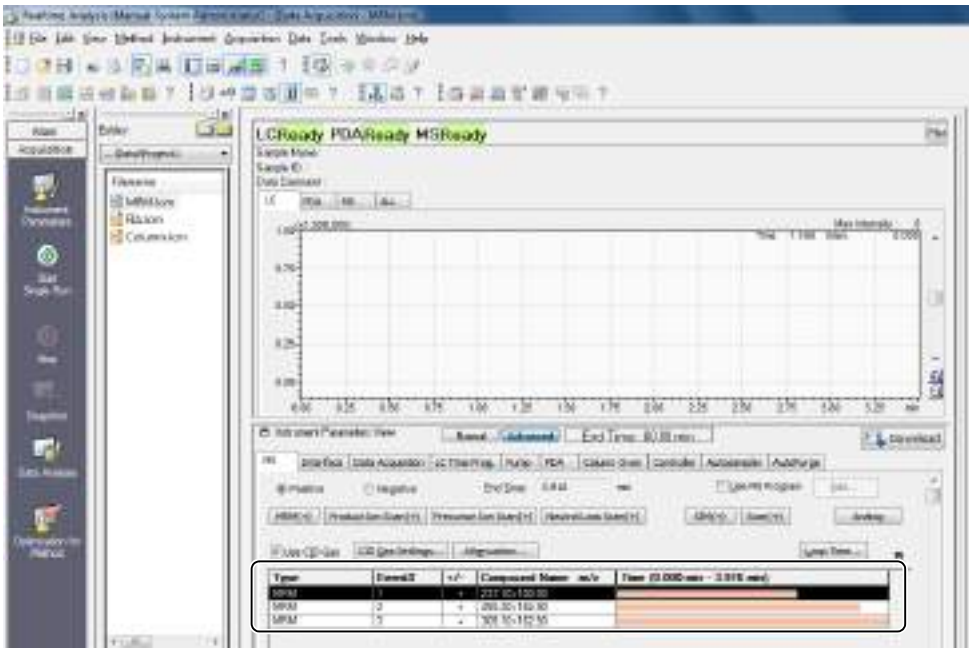


**2** **When the confirmation message is displayed, click [Yes].**

The measurement times in MRM events set in MS instrument parameters are updated.

## 9.6.3 Check Updated Results

**1** **Check measurement time update results in the Event Table.**

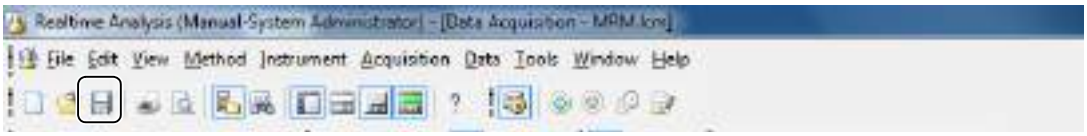


**NOTE**

- Event measurement times are calculated from retention time settings in the Compound Table and the [Process Time] settings in identification parameters.
- Measurement times for non-MRM events are not updated.

## 9.6.4 Save to Method Files

**1** **Click** **(Save) on the toolbar.**




The results of updating MRM event measurement times are saved in the method file.

This completes the method optimization process.

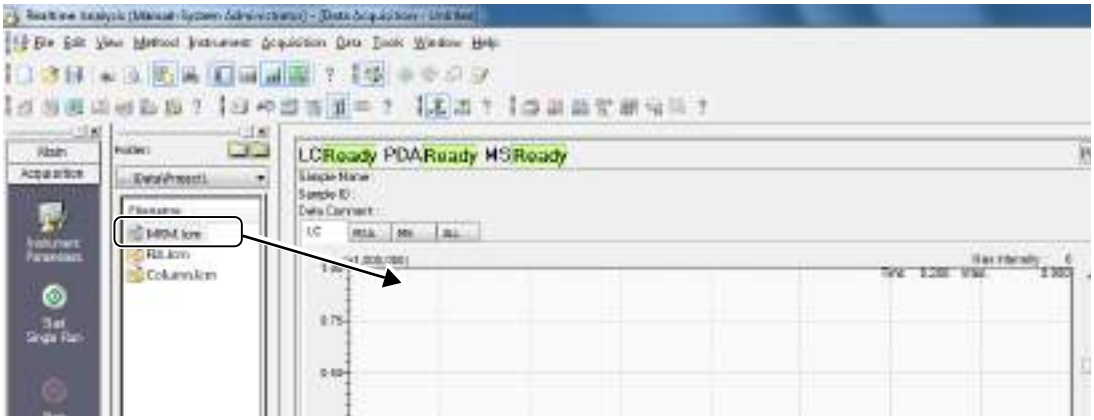
# 9.7 Create a Calibration Curve and Perform Quantitative Calculations

Use the MRM acquisition method file saved in *"9.6 Update Measurement Times in MRM Events"* to analyze the actual sample.

This section describes how to perform realtime batch on a standard sample, create a calibration curve, and quantitate an unknown sample.

## 9.7.1 Set Calibration Curve Parameters in a Method File

**1 Drag-and-drop the method file for MRM acquisition onto the [Data Acquisition] window from the [Data Explorer] sub-window.**



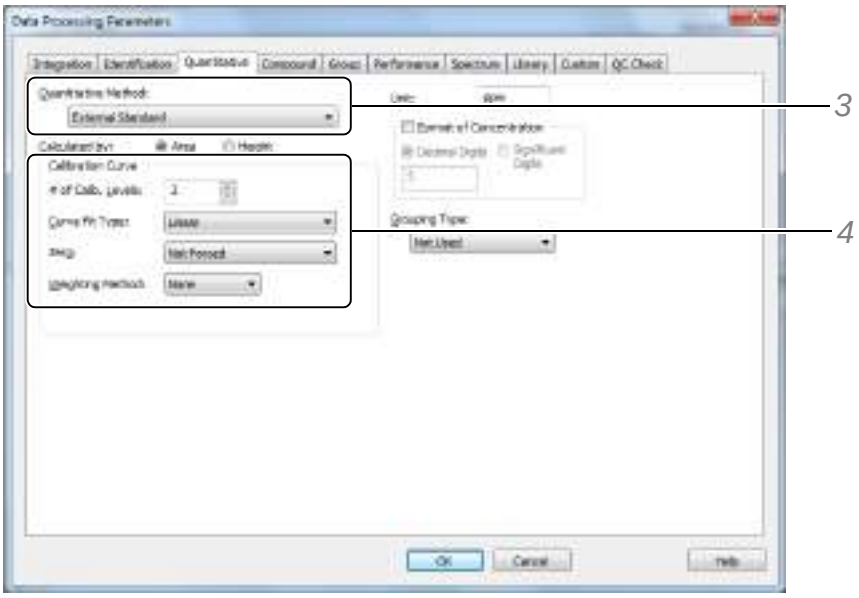

**2 Perform data acquisition on the standard sample and set parameters for creating a calibration curve.**

1 Click [Data Processing Parameters(MS)] on the [Method] menu.


The [Data Processing Parameters] sub-window is displayed.

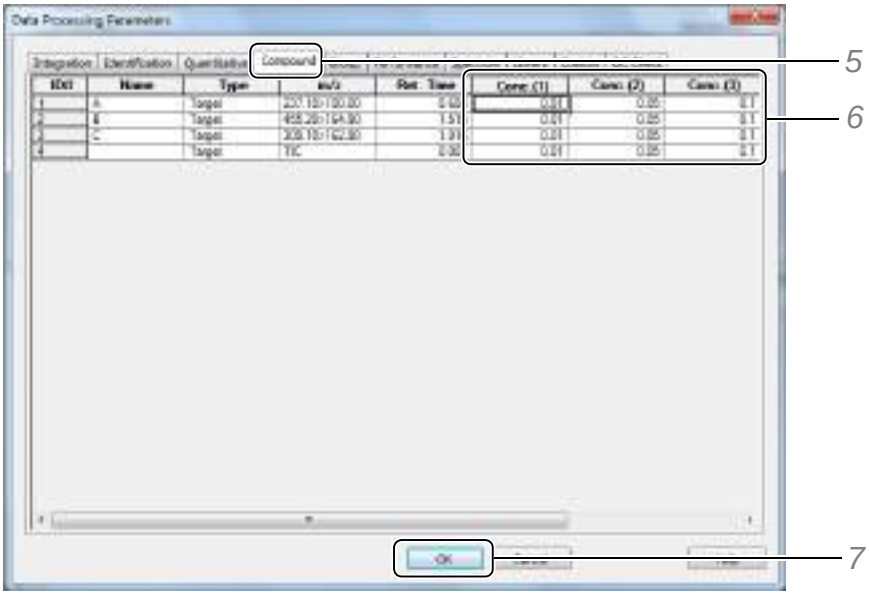
2 Click the [Quantitative] tab.

3 Select [Quantitative Method].




4 Set the number of levels and type of calibration curve.

5 Click the [Compound] tab.




6 Set the concentrations for each level of the standard sample used to create the calibration curve.

7 Click [OK] to apply the settings.

**3 Click (Save) on the toolbar.**

Quantitative processing parameters are saved in the method file for MRM acquisition.

## 9.7.2 Create a Batch Table

**1 Click the (Realtime Batch) icon on the [Main] assistant bar.**

The [Realtime Batch] window is displayed.

**2 Click the (Wizard) icon on the [Realtime Batch] assistant bar.**

The [Batch Table Wizard] sub-window is displayed.

**3 Create a Batch Table using the Batch Table Wizard.**

**Reference**

For details on operations, see *"3.2.1 Batch Table Wizard" P.43*.

| Analysis | Vial# | Tray Name | Sample Name | Sample ID | Sample Type | Analysis Type | Method File | Data File |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | | | 1:Standard:(I) | MIT MQT | MRM.lcm | Std01.lcm |
| 2 | 2 | 1 | | | 1:Standard | MIT MQT | MRM.lcm | Std02.lcm |
| 3 | 3 | 1 | | | 1:Standard | MIT MQT | MRM.lcm | Std03.lcm |
| 4 | 4 | 1 | | | 1:Standard | MIT MQT | MRM.lcm | Std04.lcm |
| 5 | 5 | 1 | | | 0:Unknown | MIT MQT | MRM.lcm | Unk01.lcm |
| 6 | 6 | 1 | | | 0:Unknown | MIT MQT | MRM.lcm | Unk02.lcm |
| 7 | 7 | 1 | | | 0:Unknown | MIT MQT | MRM.lcm | Unk03.lcm |

## 9.7.3 Start Realtime Batch

**1** **Place standard and unknown samples on the autosampler, with the trays and vial number in the order set in the Batch Table.**

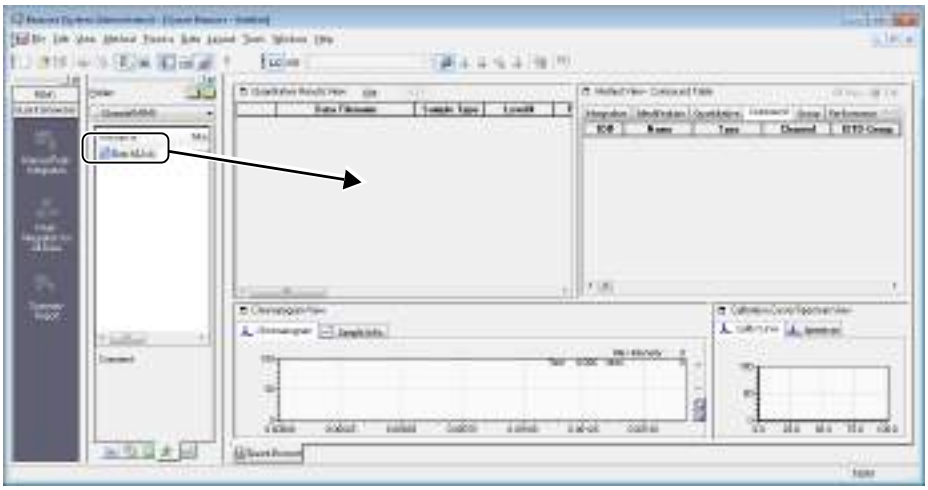
**2** **Click the**  **(Start Realtime Batch) icon on the [Realtime Batch] assistant bar.**

Realtime Batch is executed.

## 9.7.4 Check Quantitative Results in the Quant Browser

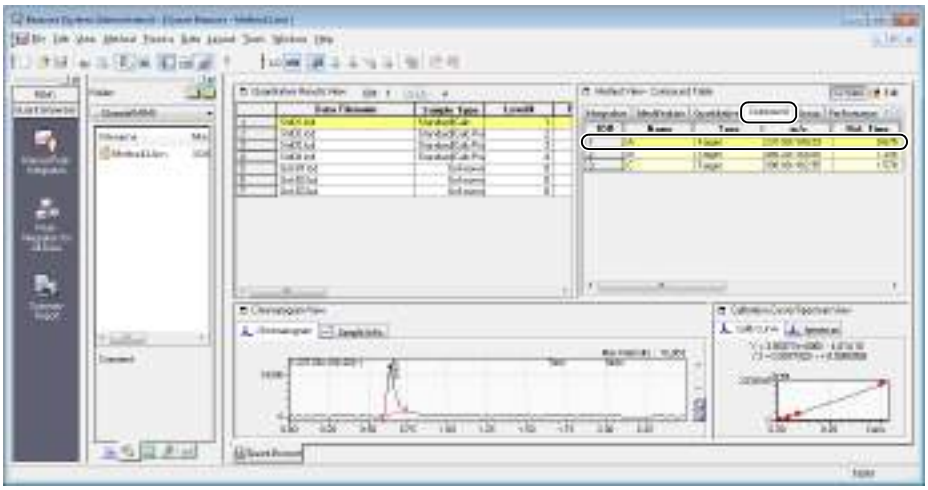
Check the quantitative results calculated in *"9.7 Create a Calibration Curve and Perform Quantitative Calculations"* in the [Quant Browser] window.

**1** **Drag-and-drop the batch file used for continuous data acquisitions onto the [Quant Browser] window from the [Batch] tab in the [Data Explorer] sub-window.**

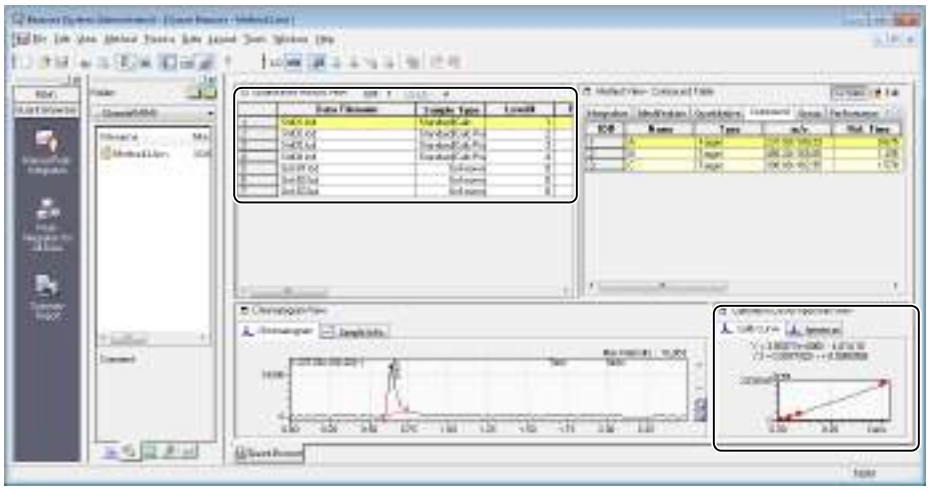


The contents of the method file and data file currently set in the batch file are displayed in the [Quant Browser] window.

**2** **Click the [Compound] tab in [Method View], and click the compound to display.**



The quantitative results of the compound selected on the [Compound] tab are displayed in [Quantitative Results View], and the calibration curve is displayed in [Calibration Curve/Spectrum View].



**Reference**

For further details, see *"11.2 Check Quantitative Results in the Quant Browser" P.330*.

# 9.8 Reoptimize Previously Optimized Methods

To re-optimize methods that have already been optimized before, use the following procedure.

## 9.8.1 Prepare the Sample

**1** **Remove the column to allow flow injection analysis.**

**2** **Place the samples on the autosampler.**

## 9.8.2 Change the Method File for Flow Injection Analysis

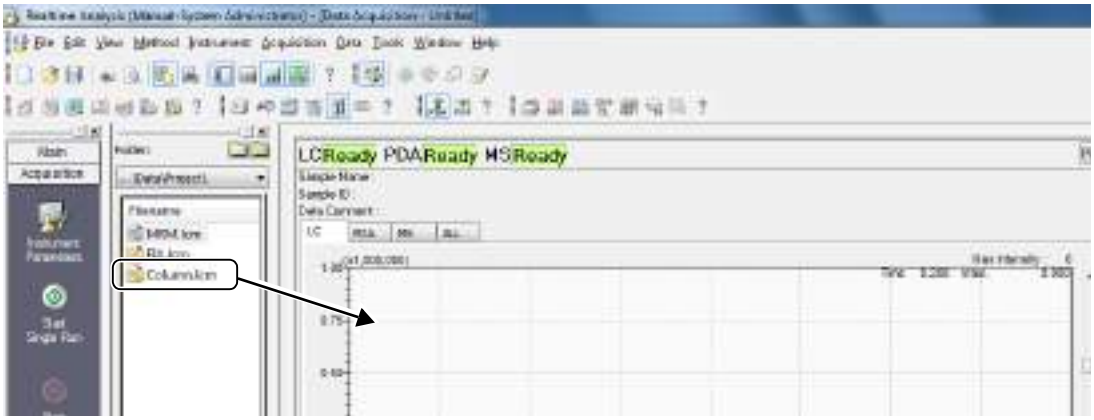
Change a previously optimized method file (for column analysis) for use in flow injection analysis.

**1** **Start up the [Realtime Analysis] program from the [LabSolutions Main] window to open the [Data Acquisition] window.**

**Reference**

For details on operations, see *"2.1.1 Open the [Data Acquisition] Window" P.9*.

**2** **Drag-and-drop the method file onto the [Data Acquisition] window from the [Data Explorer] sub-window.**



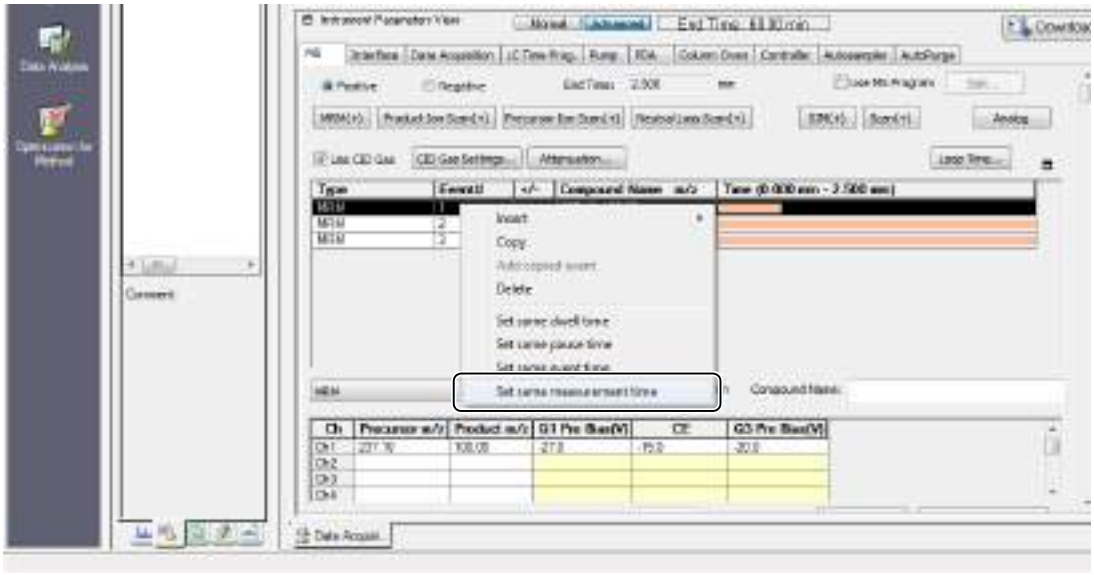

**3** **Change the LC instrument parameters for use in flow injection analysis.**

1. Change the flowrate on the [Pump] tab. (Example: 0.2 mL/min)
2. Set a short time on the [Data Acquisition] tab. (Example: 0.5 min)
3. Delete all rows except the [stop] command on the [LC Time Prog.] tab.
4. Change a time of the [stop] command on the [LC Time Prog.] tab. (Example: 0.5 min)
5. Deselect the [Column Oven] checkbox on the [Column Oven] tab.

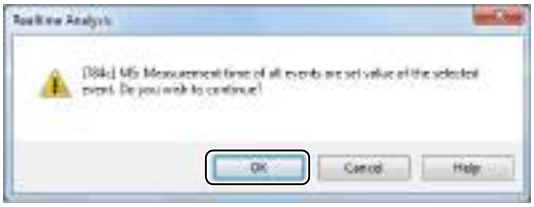
**4** **Select one of the events in MS instrument parameters, set the measurement time, and click [Set Same Measurement Time] on the right-click menu.**

**NOTE**

Since the analysis is performed without column, please set a short analysis time.




**5** **When the confirmation message is displayed, click [OK].**



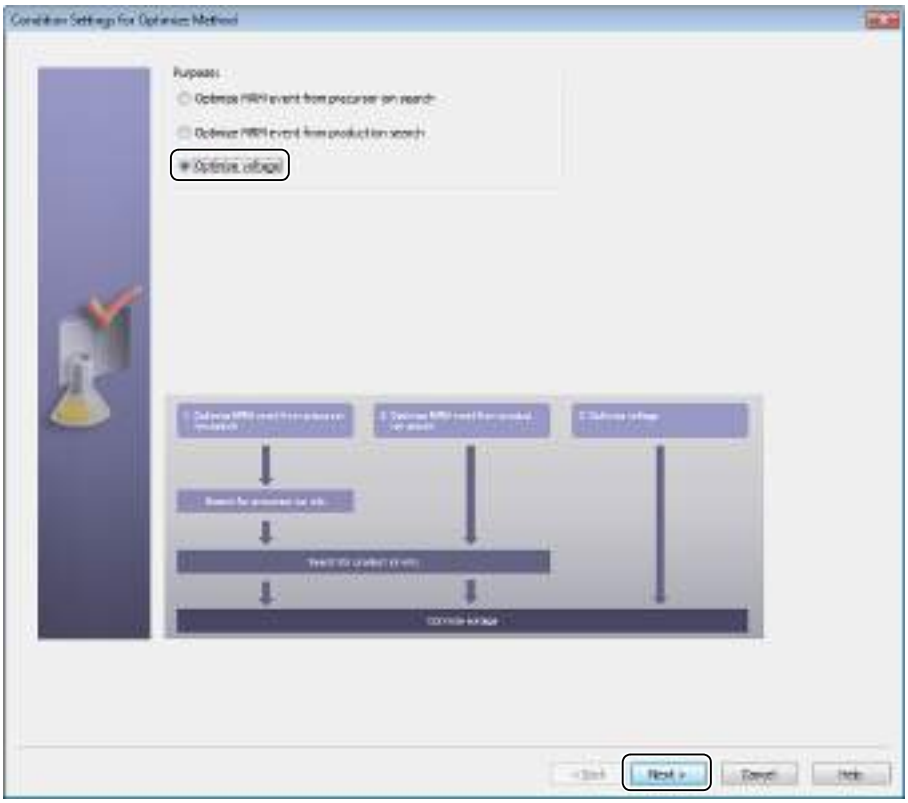

This results in the same measurement time for all events.

## 9.8.3 Optimize Method

**1** **Click the  (Optimization for Method) icon on the [Acquisition] assistant bar.**

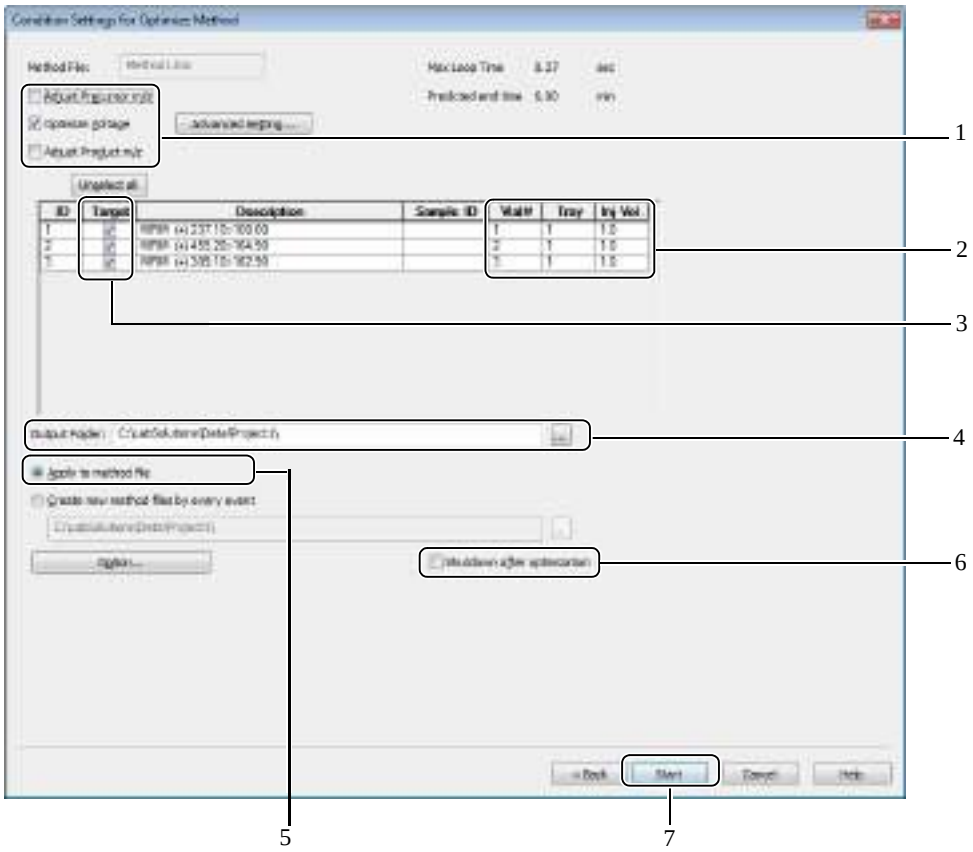
The [Condition Settings for Optimize Method] sub-window is displayed.

## 2 Click [Optimize voltage], and click [Next].



The [Condition Settings for Optimize Method] sub-window is displayed.

## 3 Set the optimization conditions, and click [Start].




Optimize each event by measuring the sample for each item selected in area 1.

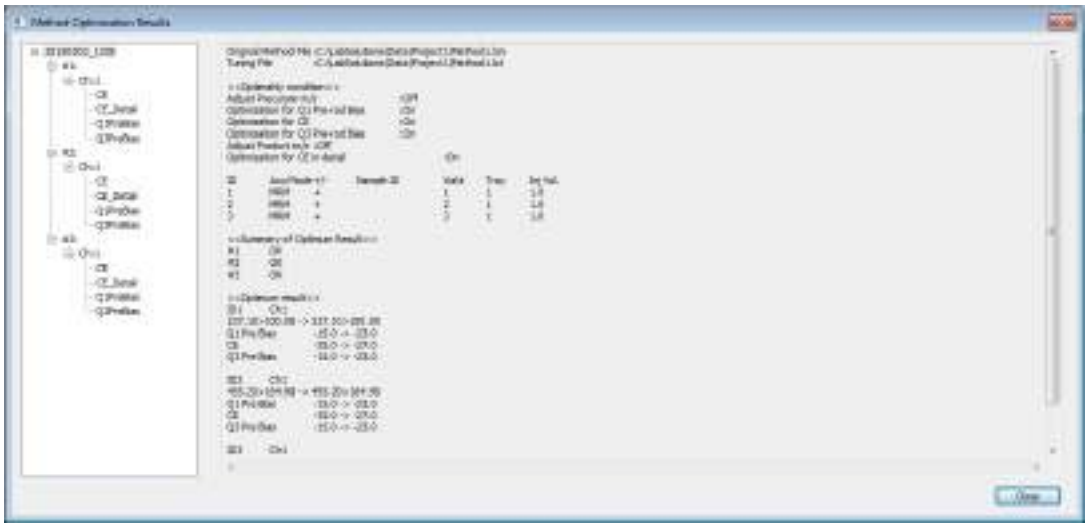
| No. | Description |
|---|---|
| 1 | When [Adjust Precursor m/z] is selected, the *m/z* value with the highest peak intensity within the -0.5 to +0.5 u range is determined for precursor ion *m/z* set in MS instrument parameters.<br>When [Optimize Voltage] is selected, the items selected for optimization in the [Optimize voltage settings] sub-window, which is displayed by clicking [Advanced Settings], are optimized.<br>When [Adjust Product m/z] is selected, the *m/z* value with the highest peak intensity within the -0.5 to +0.5 u range is determined for product ion *m/z* identified by automatic searching. |
| 2 | Enter the vial number, tray, and injection volume for samples used for optimization.<br>It indicates information about samples prepared in *"9.8.1 Prepare the Sample"*. |
| 3 | Select the events to optimize. |
| 4 | A subfolder is created under the folder specified here. The name of the subfolder is determined by the date and time. The files automatically created during the optimization are output in this folder.<br>**NOTE**<br>The default is the project folder. |
| 5 | Select [Apply to method file]. Optimized results are applied to the currently open method file. |
| 6 | When [Shutdown after optimization] is selected, realtime batch is executed after optimization is finished.<br>When performing shutdown after optimization, the method file currently opened is closed. |
| 7 | Check [Predicted end time], and click [Start]. |

**NOTE**

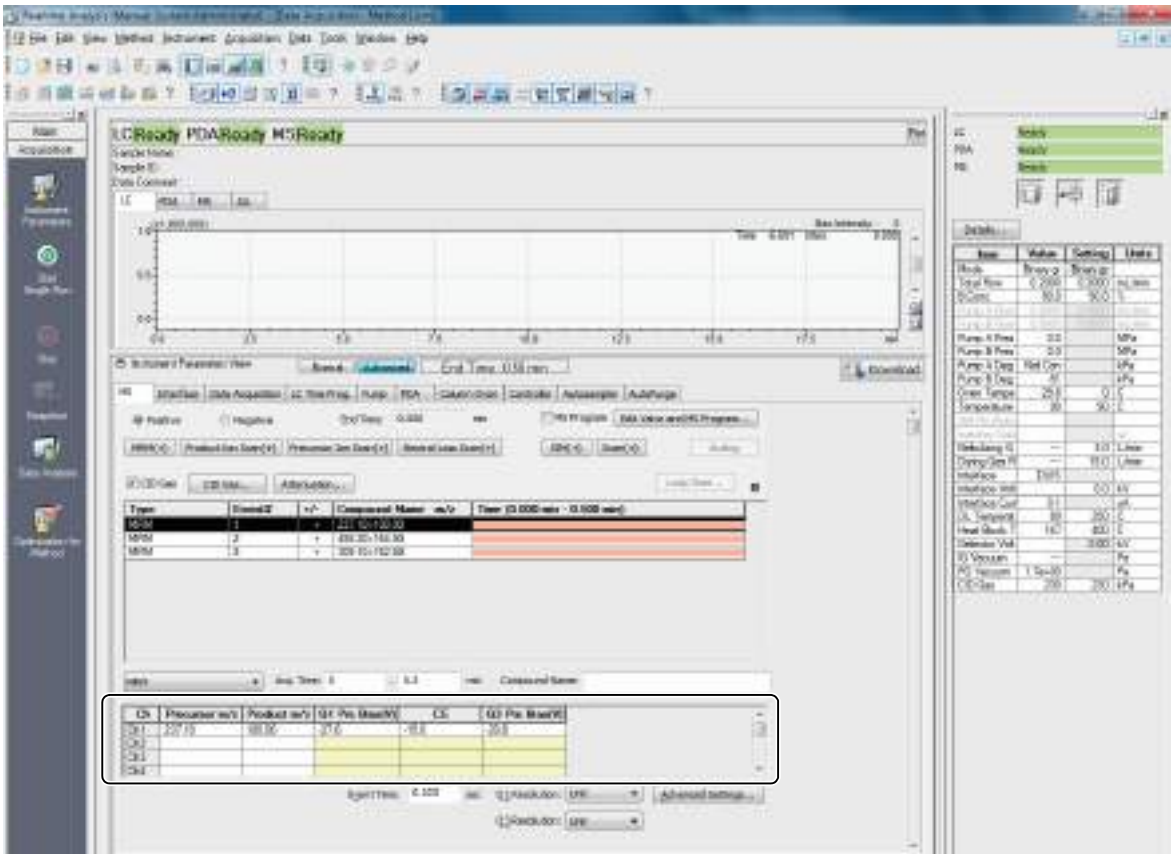
The [Proceeding for Optimize method] sub-window is displayed during optimization. Clicking [Stop] stops method optimization.

## ■ Display Optimization Results

After optimization is finished, click [Detail] in the [Proceeding for Optimize method] sub-window to display the [Method Optimization Results] sub-window.



The results are reflected in the method parameters.



**NOTE**

- The displayed items vary according to the MS detector model.
- After the [Proceeding for Optimize method] sub-window is closed, optimization results can be displayed by clicking [Optimization Result] on the [Method] menu in the [Data Acquisition] window.
- The data files output during the optimization are saved in the folder set at 4. To check detailed results, open the target data file in the [MS Data Analysis] window.



## 9.8.4 Restore Method File for Column Analysis and Confirm Retention Times

**1** **Change the LC instrument parameters for use in column analysis.**

Restore settings for column analysis, such as the pump flowrate, time program, data acquisition time, and column oven control.

**2** **Check the compound retention times by single run.**

**Reference**

For details on operations, see *"9.4 Check Compound Retention Times" P.297*.

**3** **After single run is finished, set retention times in the Compound Table.**

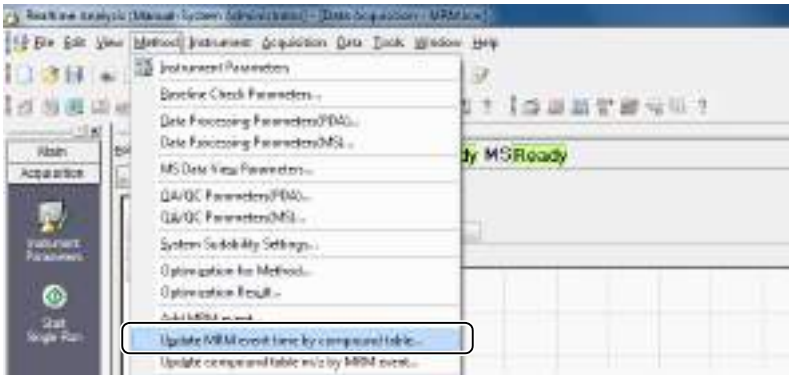
**Reference**

For details on operations, see *"9.5 Set Retention Times in the Compound Table" P.300*.

## 9.8.5 Update Measurement Times for MRM Events in Methods

Based on retention times in the Compound Table, update the measurement times for MRM events in MS instrument parameters.

**1** **Click [Update MRM event time by Compound] on the [Method] menu.**



**2** **When the confirmation message is displayed, click [Yes].**

The measurement times for MRM events in MS instrument parameters are updated.

That completes the method optimization process.

# 10 Automatic MS/MS

Automatic MS/MS measurements are used when observed ions are unknown. Precursor ions are selected and MS/MS analysis is performed automatically according to criteria settings.

**NOTE**

If the LCMS-8030, LCMS-8040, LCMS-8045, LCMS-8050 or LCMS-8060 is used as an MS detector, automatic MS/MS measurement is enabled.

## 10.1 Perform Measurements by Automatic MS/MS

This section describes how to automatically measure samples by MS/MS, using the Q3 scan for survey events (parent events) and the product ion scan for dependent events (child events).

**1** **Start up the [Realtime Analysis] program from the [LabSolutions Main] window to open the [Data Acquisition] window.**

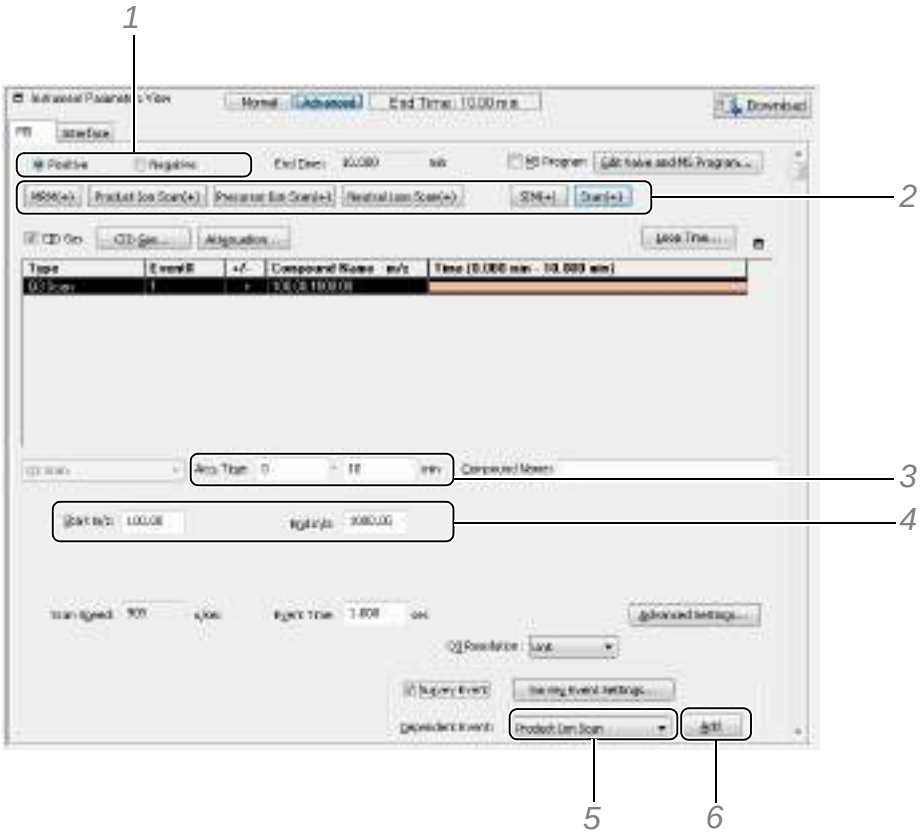
**Reference**

For details on operations, see *"2.1.1 Open the [Data Acquisition] Window" P.9*.

**2** **Click the [MS] tab.**

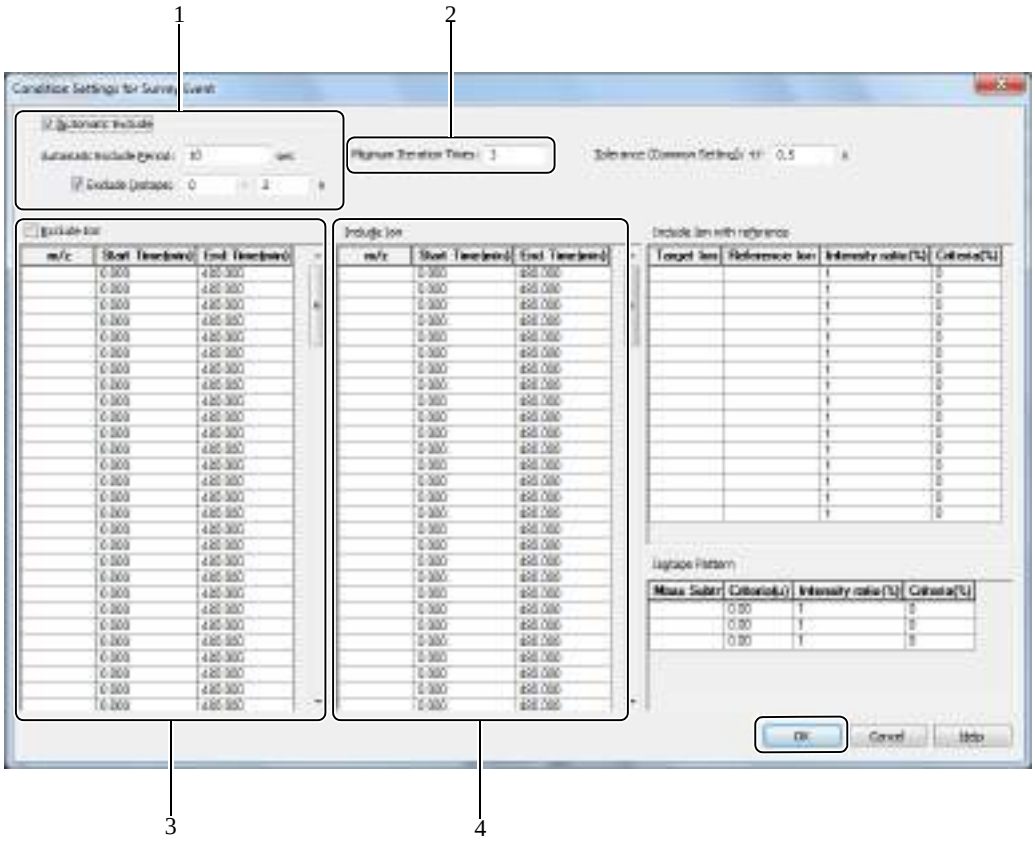
## 3 Set the survey event.

Add the survey event to the Event Table and set measurement conditions.




1 Select the event polarity.
2 Click the button for the event's data acquisition mode.
The event with the initial settings is added to the Event Table.
3 Set the measurement time.
4 Set the *m/z* range to measure.
5 Select [Use as Survey Event].
6 Click the [Survey Event Settings] button.
The [Condition Settings for Survey Event] sub-window is displayed.

## 4 Set the execution conditions for the survey event.




| No. | Description |
|---|---|
| 1 | Selecting [Automatic Exclude] automatically excludes previous precursor ions and prevents them from being selected as precursor ions for the period set at [Automatic Exclude Period]. |
| 2 | Set the minimum repeat counts (count that is repeated even if the result of the survey event is weak) for dependent events that use the same mass. |
| 3 | Set the *m/z* values and measurement time to exclude in selecting ions as precursors. |
| 4 | Set the *m/z* values and measurement time to prioritize in selecting ions as precursors. |

**Reference**

For details on how to set this sub-window, refer to Help.

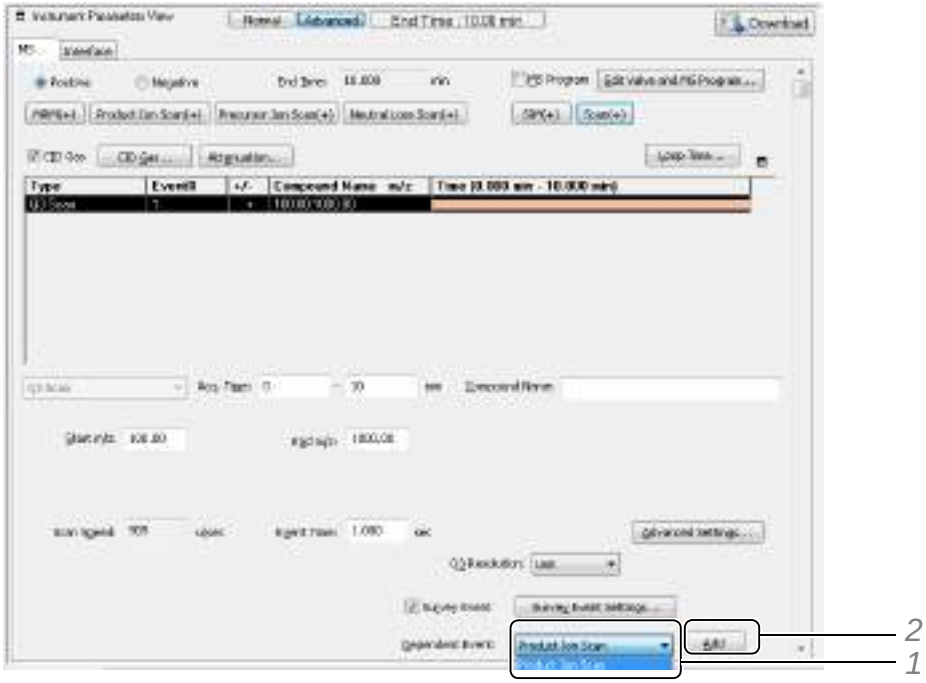
## 5 Click [OK].

This returns to the original sub-window.

## 6 Set the dependent event.

Add the dependent event to the Event Table and set measurement conditions.

1 Select the data acquisition mode for the dependent event.
2 Click the [Add] button.

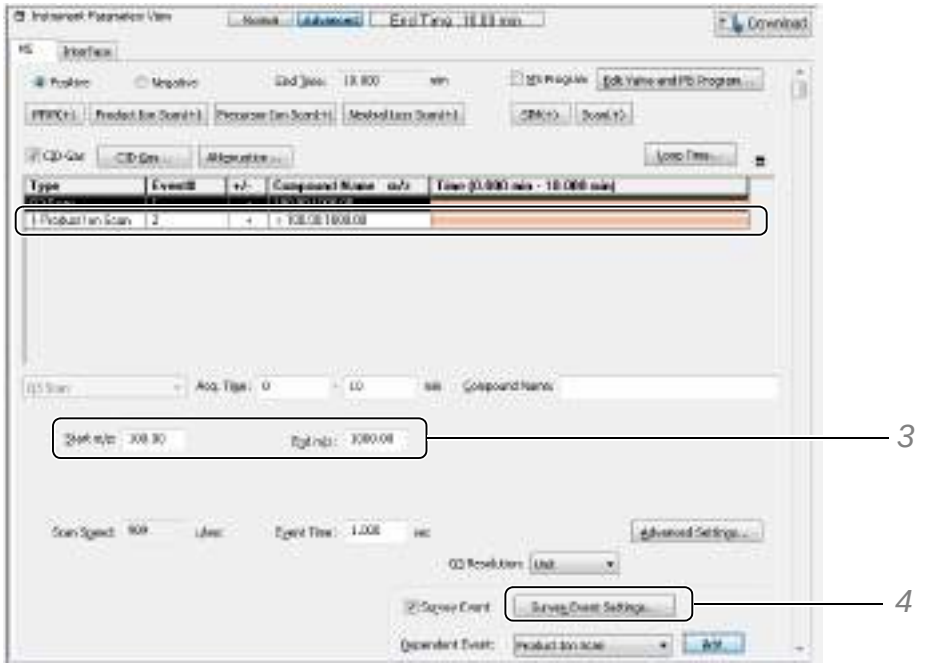



A corresponding dependent event is added to the survey event in the Event Table.

**NOTE**

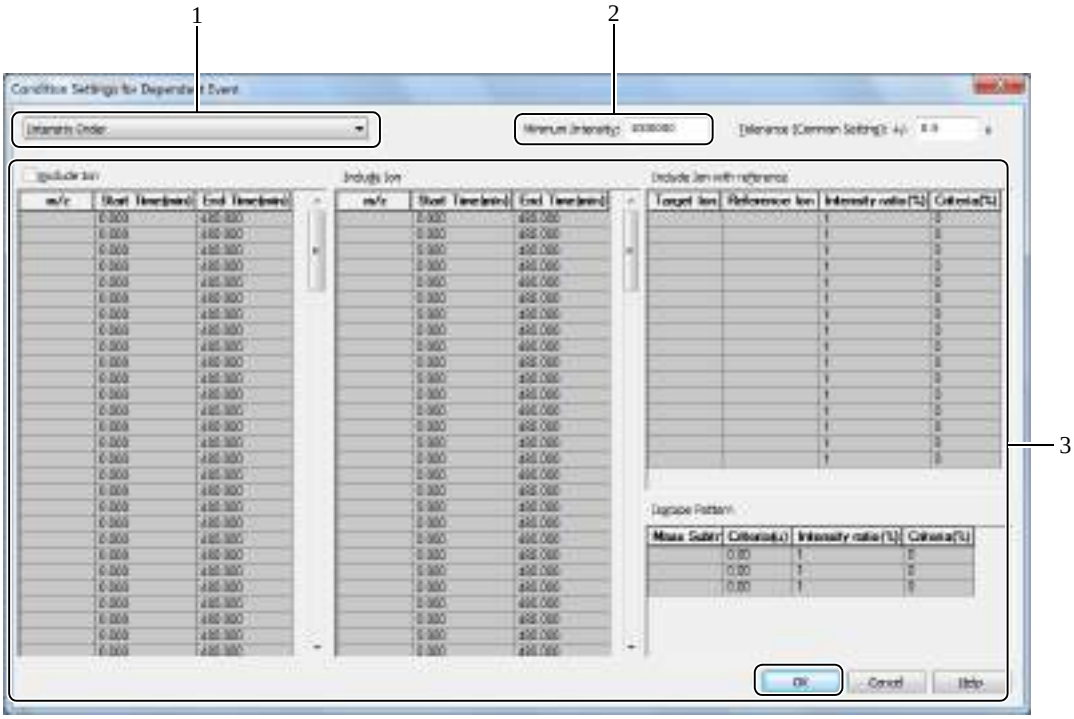
The polarity and measurement time range is the same as for the survey event.

3 Set the *m/z* range to measure.
4 Click the [Dependent Event Settings] button.




The [Condition Settings for Dependent Event] sub-window is displayed.

## 7 Set the execution conditions for the dependent event.




| No. | Description |
|---|---|
| 1 | Set the criteria for dependent events in selecting precursor ions. |
| 2 | Enter the minimum intensity value (absolute intensity) for precursor ions, where ions with lower intensity are excluded. |
| 3 | Displays the settings made in the [Condition Settings for Survey Event] sub-window. These items cannot be edited in this sub-window. |

**Reference**

For details on how to set this sub-window, refer to Help.

## 8 Click [OK], and close the [Condition Settings for Dependent Event] sub-window.

## 9 Click the (Start Single Run) icon on the [Acquisition] assistant bar.

## 10 Set the data acquisition settings, and click [OK].

**Reference**

For details on operations, see *"2.5.1 Execute Single Run" P.36* .

# 10.2 Check Data Measured by Automatic MS/MS

This section describes how to display automatic MS/MS measurement results in the [MS Data Analysis] window.

## 10.2.1 Load Data Files

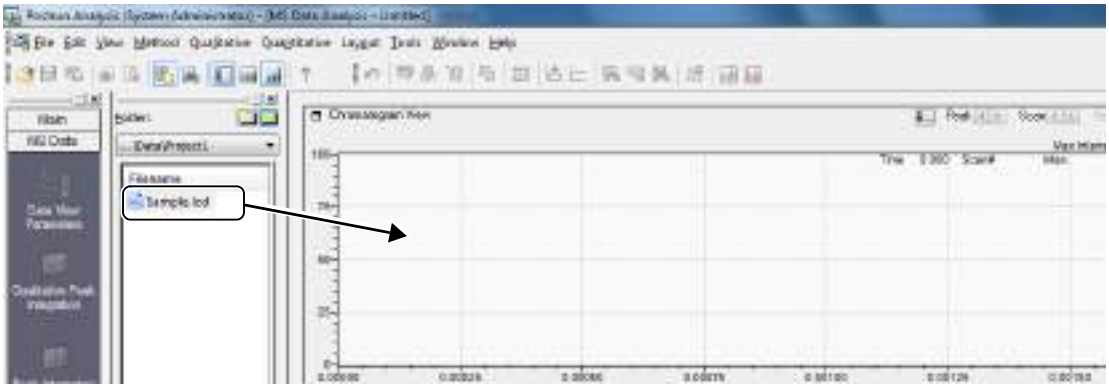
**1** **Click the  (Data Analysis) icon on the [Acquisition] assistant bar to open the [MS Data Analysis] window.**

**Reference**

For details on how to use the [MS Data Analysis] window, see *"6.1.1 Open the [MS Data Analysis] Window" P.175*.

The [MS Data Analysis] window is displayed.

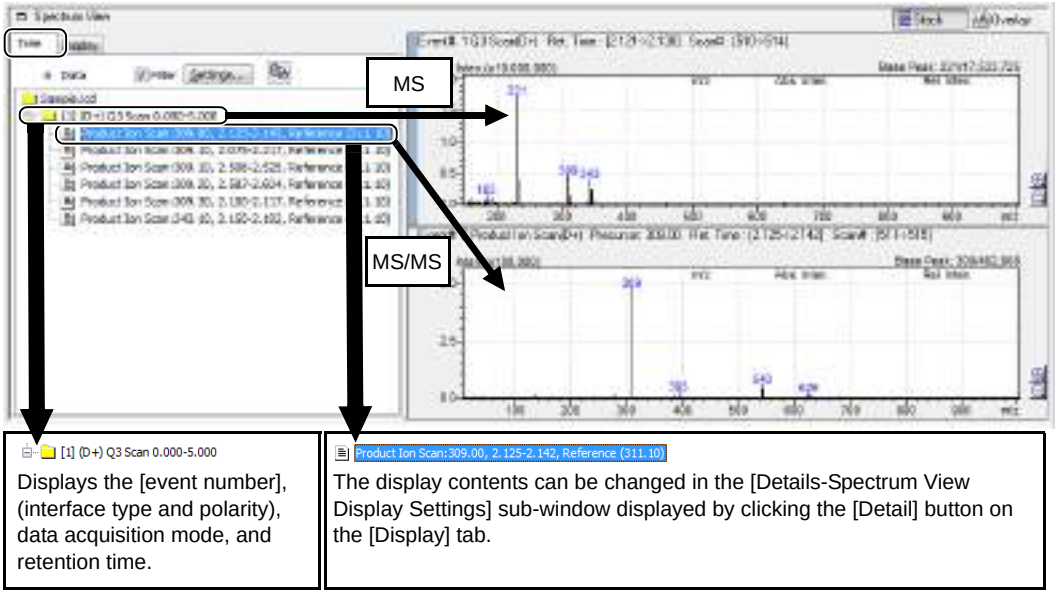
**2** **Drag-and-drop the data file acquired in *"10.1 Perform Measurements by Automatic MS/MS"* onto the [MS Data Analysis] window from the [Data Explorer] sub-window.**



The content of the data file is displayed in the [MS Data Analysis] window.

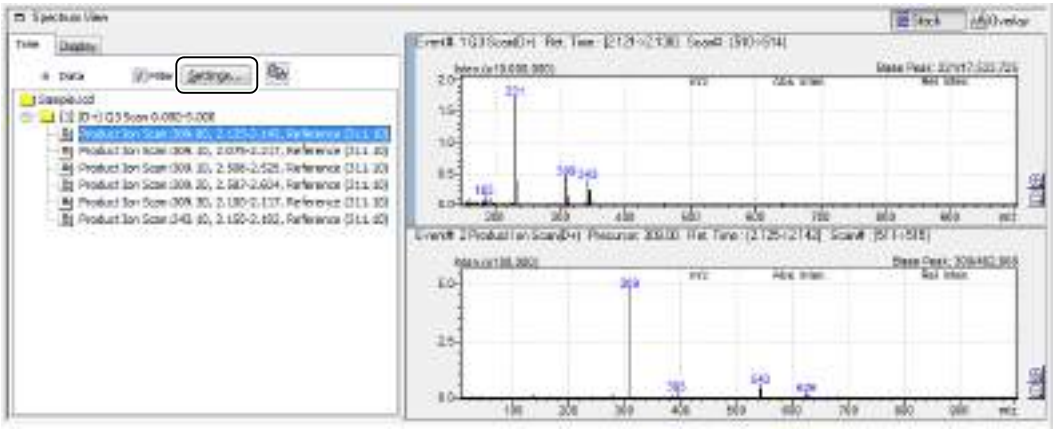
**3** **Click the [Tree] tab in [Spectrum View].**

Selected precursor ions are displayed on the [Tree] tab in [Spectrum View], in order of m/z. Clicking a precursor ion listed in the tree displays corresponding spectra of survey and dependent events.




## 10.2.2 Change the Tree Display Content

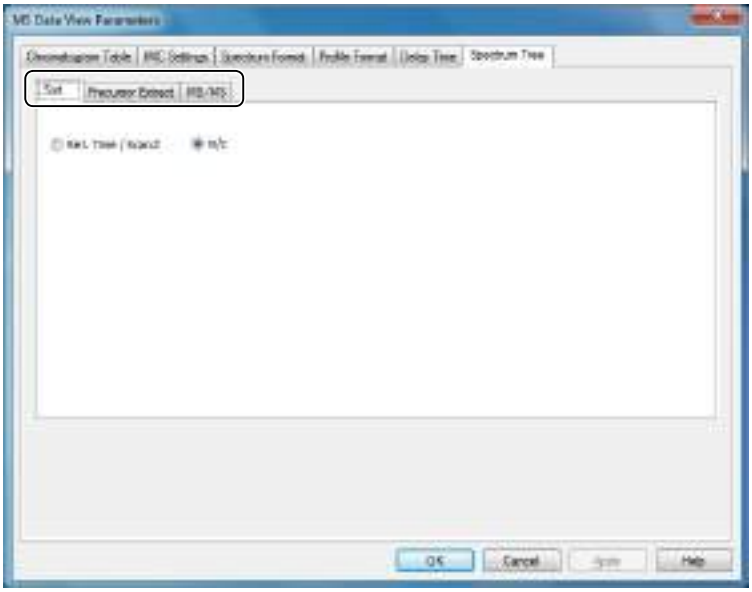
**1** **Click the [Settings] button on the [Tree] tab in [Spectrum View].**



The [MS Data View Parameters] sub-window is displayed. This sub-window allows setting detailed spectrum tree display settings.

## 2 Switch between editing sub-windows by clicking on respective tabs on the [Spectrum Tree] tab.

The tree display can be updated without closing the sub-window by clicking the [Apply] button located on each tab.



| Items | Description |
|---|---|
| [Sort] tab | Sets the conditions for sorting items to display in tree. |
| [Precursor Extract] tab | Sets the precursor ion extraction criteria. |
| [MS/MS] tab | Edits the precursor ion masses. Allows detailed filtering of precursor ions to display in the tree. |

### Reference

For details on how to set the parameters for each tab, refer to Help.

# 11 Quant Browser

Use the [Quant Browser] window to edit a method file and then perform quantitative calculation on multiple data.

This chapter describes how to edit the quantitative results for multiple data files, and perform collective postrun analysis on multiple data files.

## 11.1 [Quant Browser] Window

The [Quant Browser] window is comprised of the following views:

- [Quantitative Results View] - displays the quantitative calculation results
- [Method View] - displays the method file parameters
- [Chromatogram View] - displays the chromatograms and sample information
- [Calibration Curve/Spectrum View] - displays the calibration curves and spectra

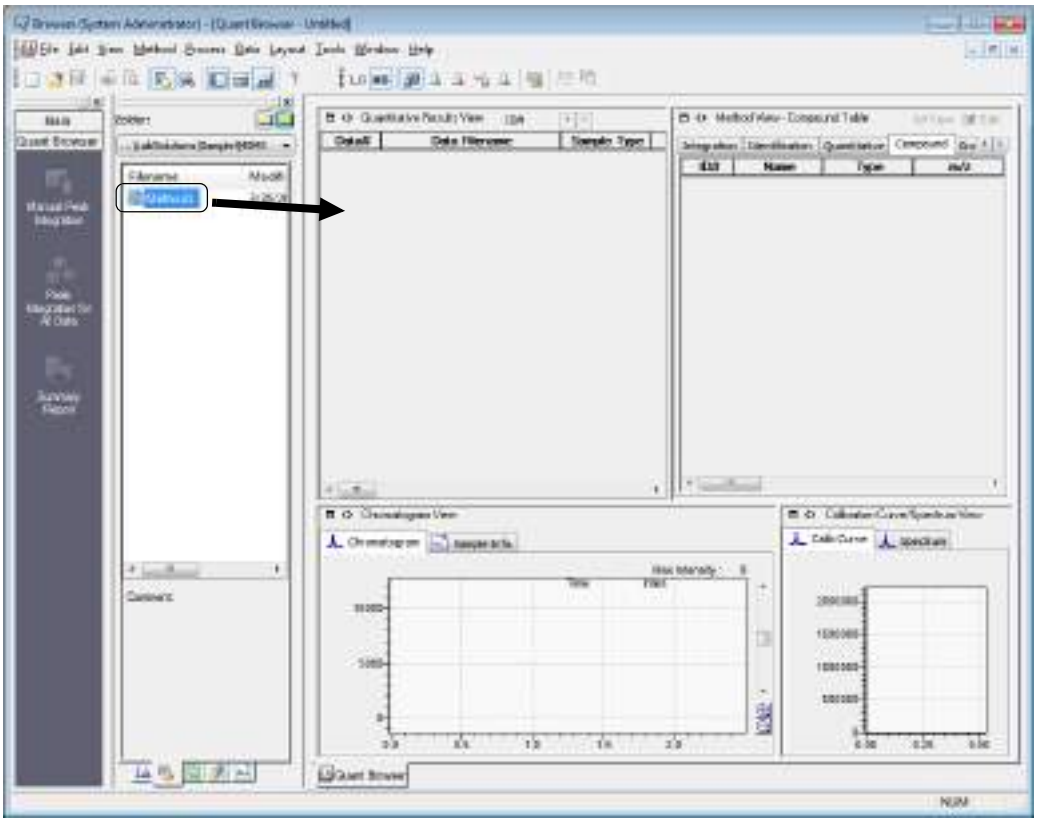
### 11.1.1 Open the [Quant Browser] Window

1 **Select the**  **icon on the [LabSolutions Main] icon bar, and double-click the**  **icon.**

The [Browser] program opens.

**2** **Click the (Quant Browser) icon on the [Main] assistant bar in the [Browser] program.**

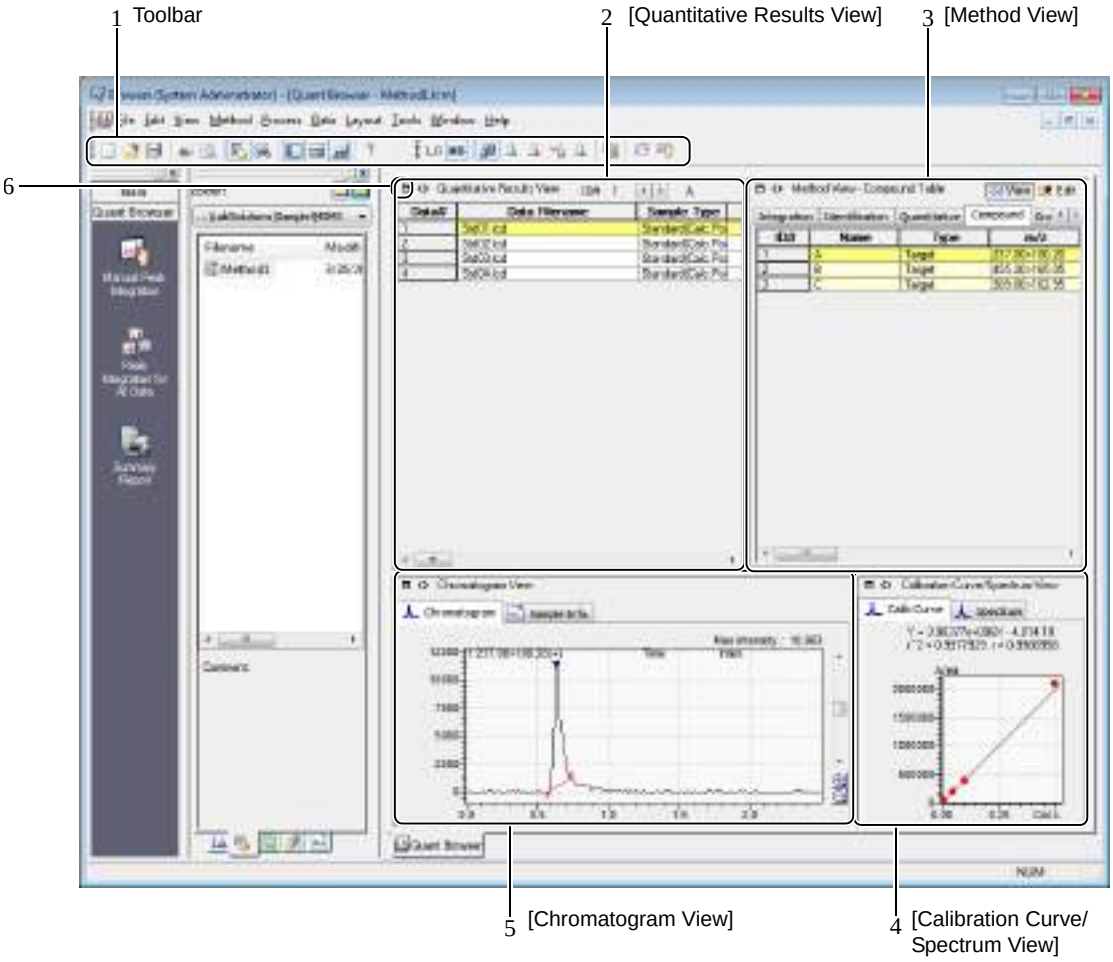
**3** **Drag-and-drop the method file from the [Data Explorer] sub-window onto the [Quant Browser] window.**



The contents of the method file are displayed in the [Quant Browser] window.

## 11.1.2 [Quant Browser] Window Description

This section describes how to view and use the [Quant Browser] window.




| No. | Explanation |
|---|---|
| 1 | Displays the [Standard] and [Quant Browser] toolbars. |
| 2 | Displays the quantitative calculation results of compounds selected on the [Compound] tab in [Method View]. Click ◀ ▶ to change the ID # and the displayed compound. |
| 3 | Displays the data processing parameters in the method file. Click Edit (Edit Mode) to change the parameters. Click View (View Mode) after editing to reflect the changes in [Method View]. |
| 4 | Displays the calibration curve for the compound selected on the [Compound] tab in [Method View] or the spectra specified in [Chromatogram View]. |
| 5 | Displays the [Chromatogram] and [Sample Info] for the selected data file. Clicking ⊕ or ⊖ to double or halve the intensity axis (Y-axis), respectively. |
| 6 | Click this icon to expand the view to the full screen size. |

**NOTE**

- The [Quant Browser] views that are separated by dividers. Drag the dividers with the mouse to resize the views.
- Use the [Quant Browser] to check the quantitative calculation results of up to 1024 data files.
- Click [Save Browsing File As] on the [Layout] menu to save the name of the method and data file, file sort order, layout information, and other details as a browsing file (file extension *.lcq).
- Files are [Read Only] if they are currently being edited in other windows and cannot be edited. Close the file in the other window, and open the file again to edit these files.

# 11.2 Check Quantitative Results in the Quant Browser

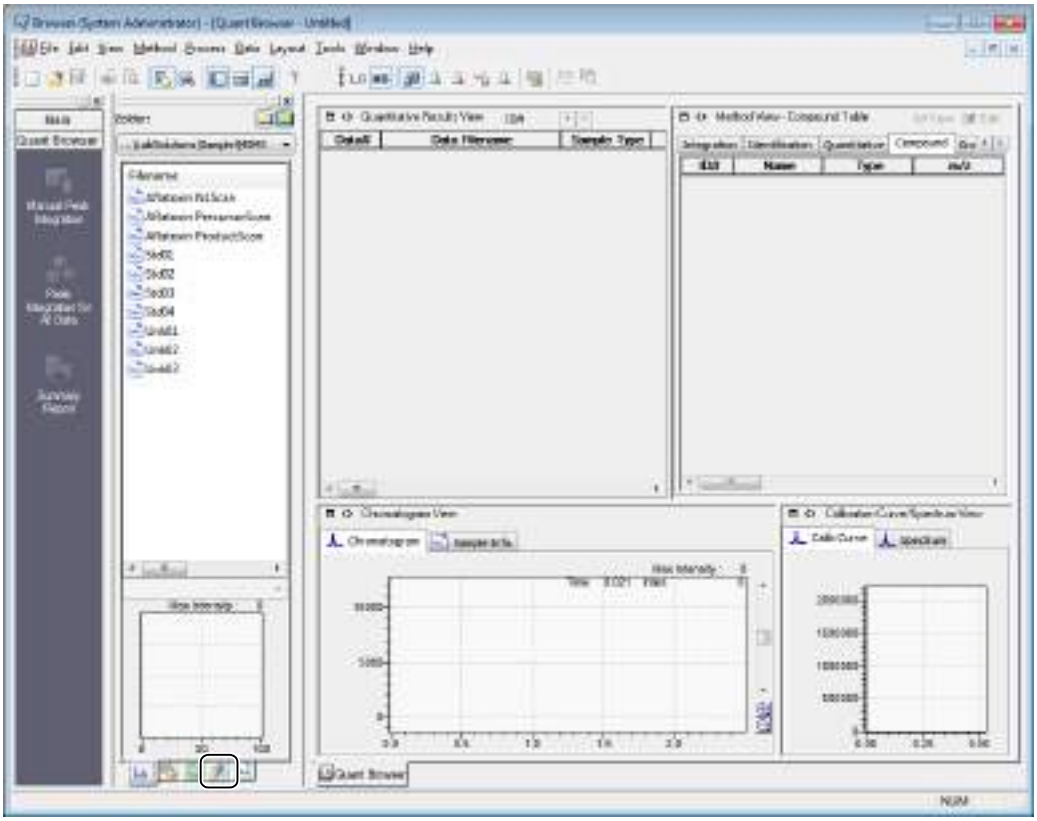
Multiple data can be displayed in a simple form in the [Quant Browser] window.

This section describes how to display data in each of the [Quant Browser] views.

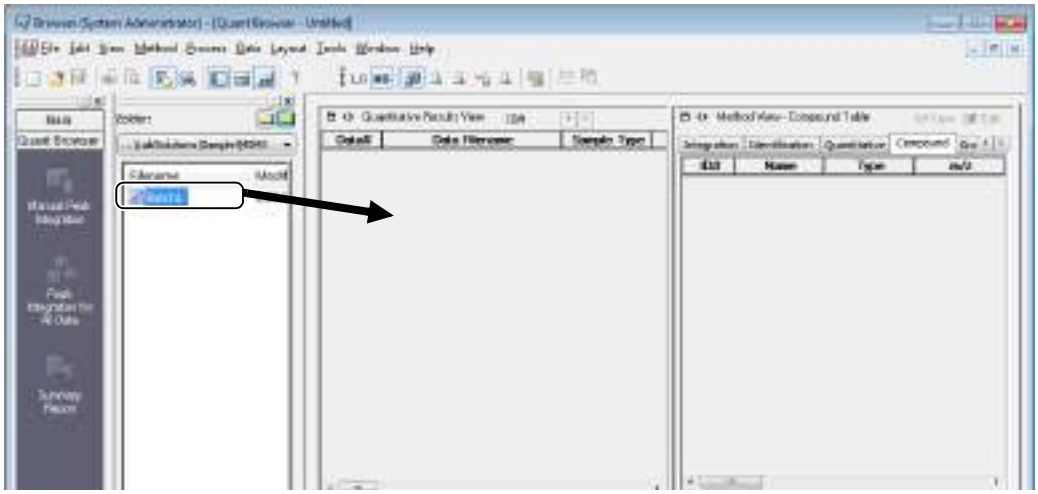
## 11.2.1 Open Batch Files

This section describes how to open batch files to display the contents of the method file and data files.

**1** **Click the (Batch) tab at the bottom of the [Data Explorer] sub-window.**



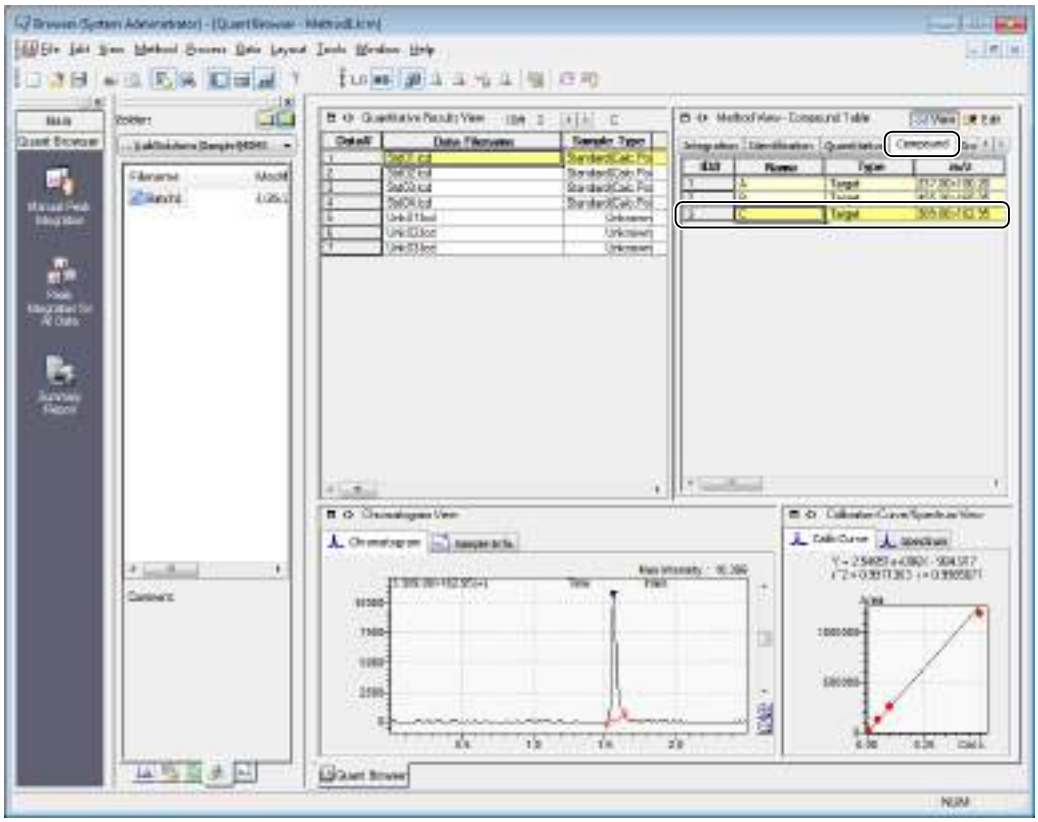
## 2 Drag-and-drop the batch file onto the [Quant Browser] window from the [Data Explorer] sub-window.



The contents of the method file and data files are displayed in the [Quant Browser] window.

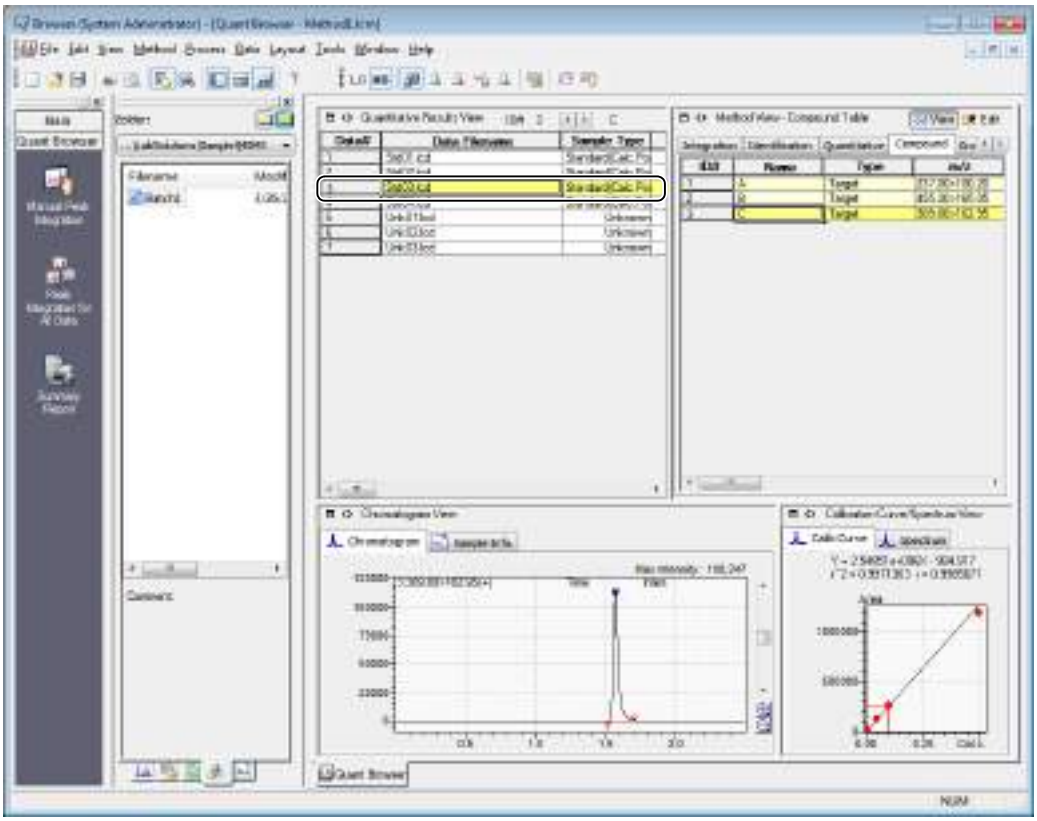
## 3 Click the [Compound] tab in [Method View], and select the desired compound.

The quantitative results of the selected compound are displayed in [Quantitative Results View], and the calibration curve is displayed in the [Calibration Curve/Spectrum View].



## 4 Select the data file from [Quantitative Results View], and click the data file.

The chromatogram of the selected data file is displayed in the [Chromatogram View].



**NOTE**

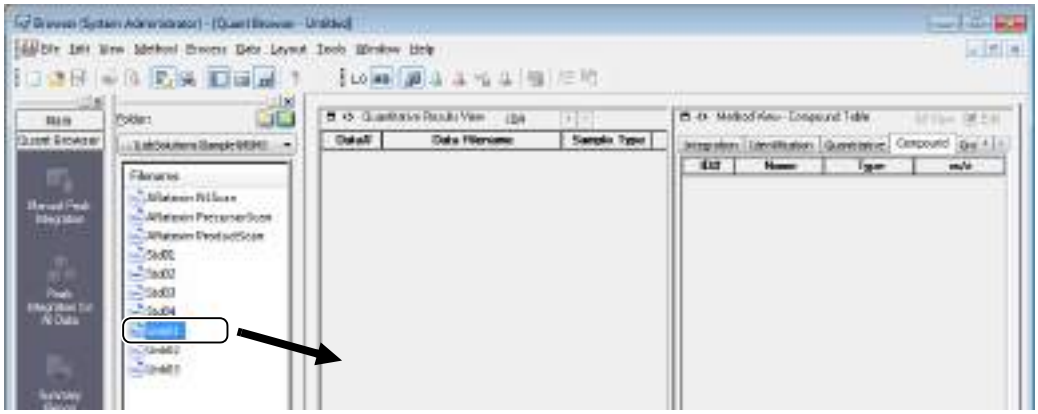
- The method file in the top row of the Batch Table is displayed in [Method View] when a batch file is selected in the [Data Explorer] sub-window. If the method file contains calibration curve information, the standard sample data file used for making the calibration curve is loaded.
- The data file and method file must be saved to the same folder as the batch file to display the content of the method file and data file using a batch file.
- Edit the method file and data file in the [Quant Browser] window. The batch file is not changed when data is displayed.

## 11.2.2 Open Data Files

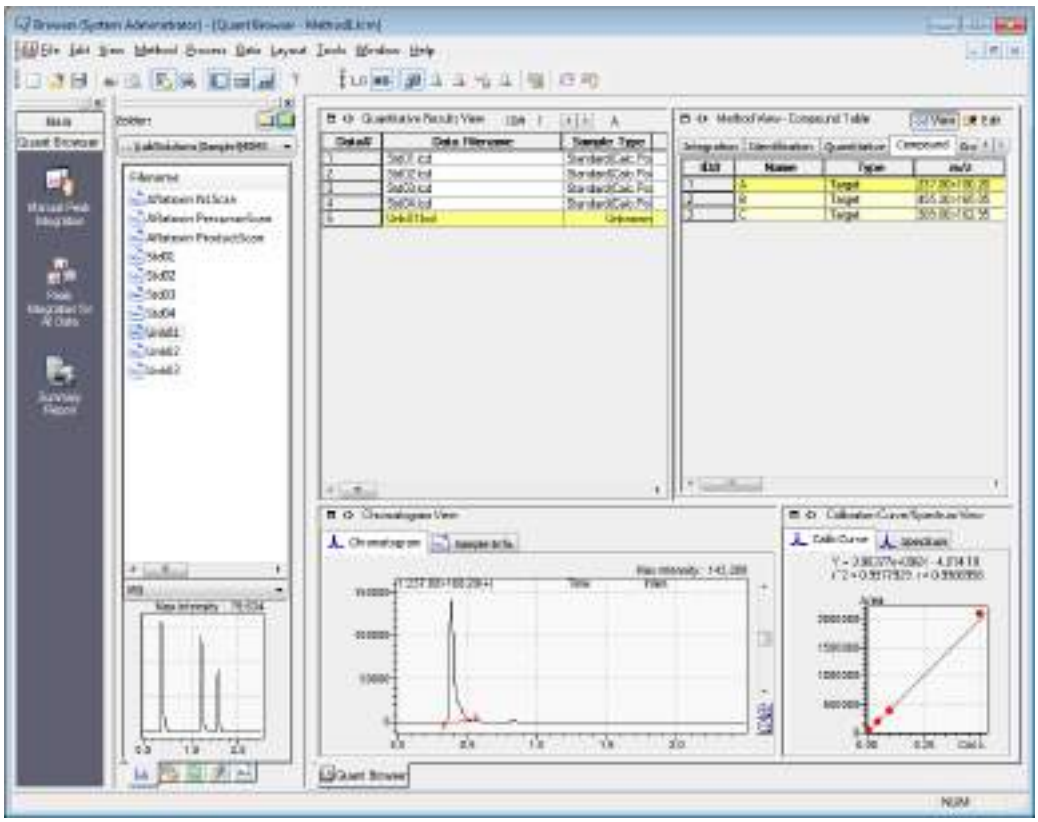
Open data files to display the contents of data files in each view.

This section describes how to open the data file of an unknown sample.

**1** **Drag-and-drop the data file onto the [Quant Browser] window from the [Data Explorer] sub-window.**



The contents of the data file and method file are displayed in the [Quant Browser] window.



**NOTE**

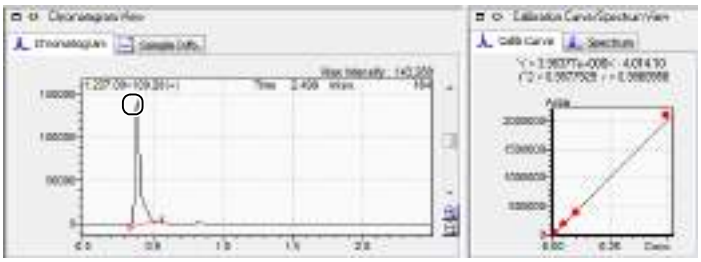
Multiple files are selected when the data file is dragged-and-dropped onto the [Quant Browser] window from the [Data Explorer] sub-window. The method file in the top data file is displayed in [Method View]. If the loaded method file contains calibration curve information, the content of the standard sample data file used to make the calibration curve is also displayed.

## 11.2.3 Check Spectra from [Chromatogram View]

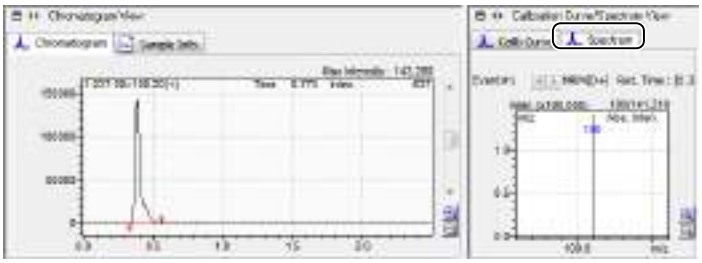
Double-click the MS or PDA chromatogram displayed in [Chromatogram View] to display the spectrum at that retention time.

This section describes how to display a MS spectrum.

**1** **Select the [Chromatogram] tab in [Chromatogram View], and double-click the MS chromatogram.**



[Calibration Curve/Spectrum View] changes to the [Spectrum] tab, and the MS spectrum is displayed.



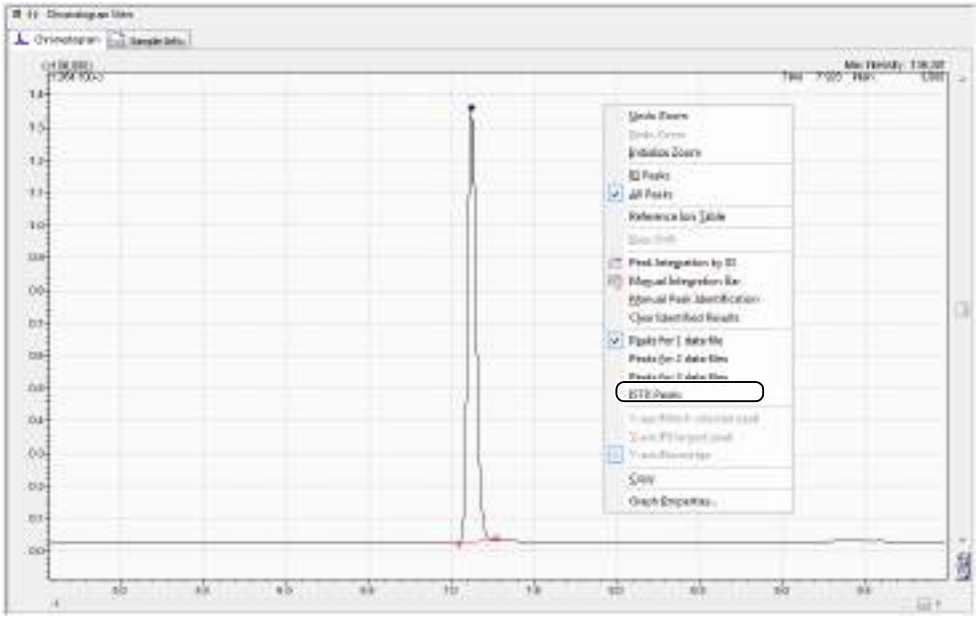
**NOTE**

- MS spectra cannot be displayed when is displayed on the MS chromatogram.
- To display chromatograms in all time ranges in [Chromatogram View], right-click on [Chromatogram View], and click [All Peaks] on the displayed menu.

## 11.2.4 Check Internal Standard Peaks

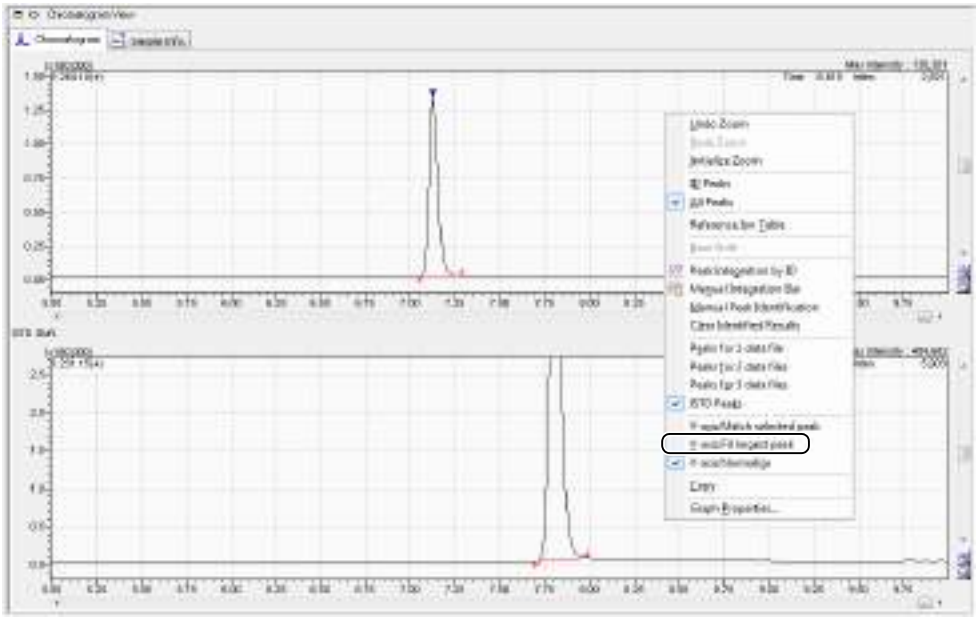
Chromatograms of ISTDs registered in the same ISTD group as the selected compound can be displayed in a stack in [Chromatogram View]. This section describes how to display ISTD chromatograms and how to adjust the scales of the Y-axes to the largest peak.

**1** **Right-click on the chromatogram on the [Chromatogram] tab page in [Chromatogram View], and click [ISTD Peaks] on the displayed menu.**

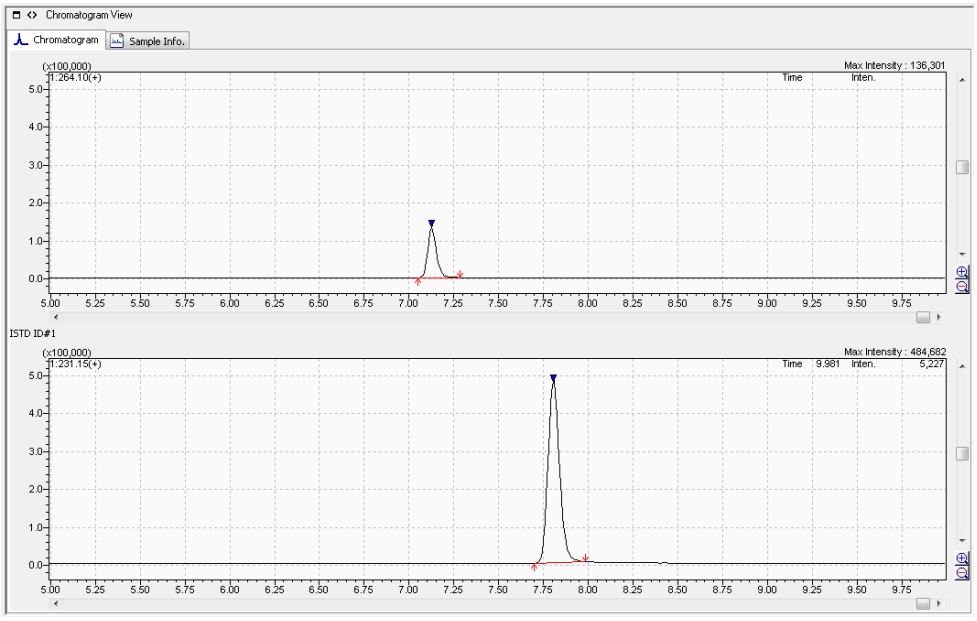


Chromatograms of ISTDs registered in the same ISTD group as the compound selected in [Compound Table] are displayed in a stack.

**2** **Right-click on the chromatogram, and click [Y-axis:Fit Largest peak] on the displayed menu.**



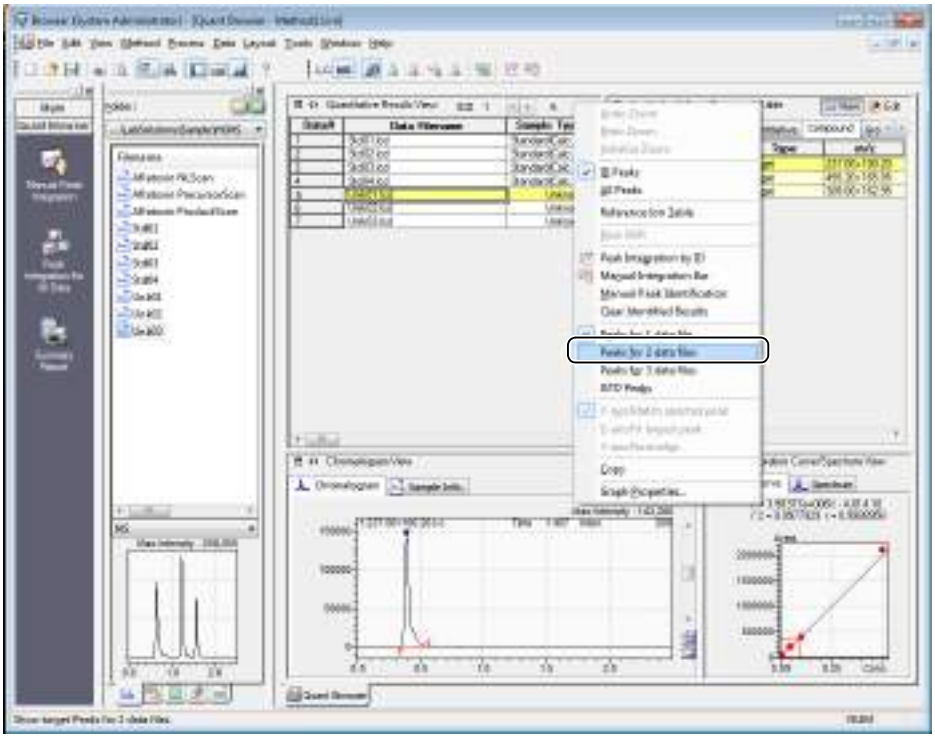
The scales of the Y axes in all the graphs are adjusted to the largest peak intensity in the displayed graphs.



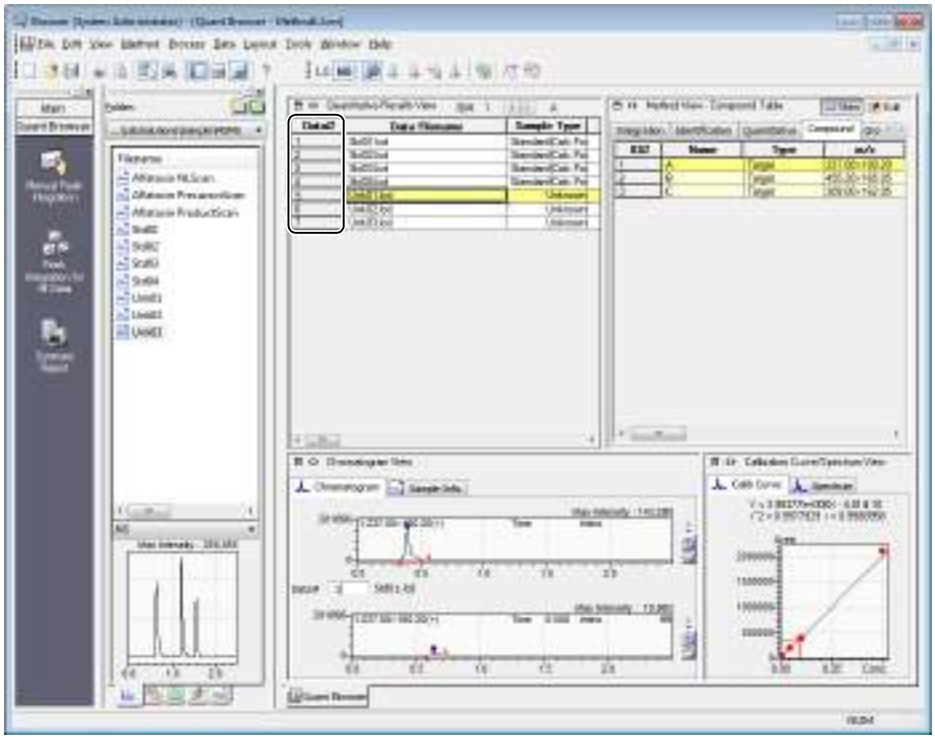

## 11.2.5 Display Chromatograms from Multiple Data

Chromatograms from the multiple data files can be displayed in [Chromatogram View] in a stack. This section describes how to display the chromatograms from two data files.

**1** **Right-click on the chromatogram on the [Chromatogram] tab page in [Chromatogram View], and then click [Peaks for 2 data files] on the displayed menu.**



**2** **Enter the [Quantitative Results View]-[Data#] number that corresponds to the data file to display, at [Data#] in [Chromatogram View].**



Chromatograms that have the same ID numbers as the compounds selected in [Compound Table] are displayed in a stack.

# 11.3 Postrun Analysis of Multiple Data

This section describes how to edit [Quantitative Results View] and [Method View] and perform collective postrun analysis on multiple data.

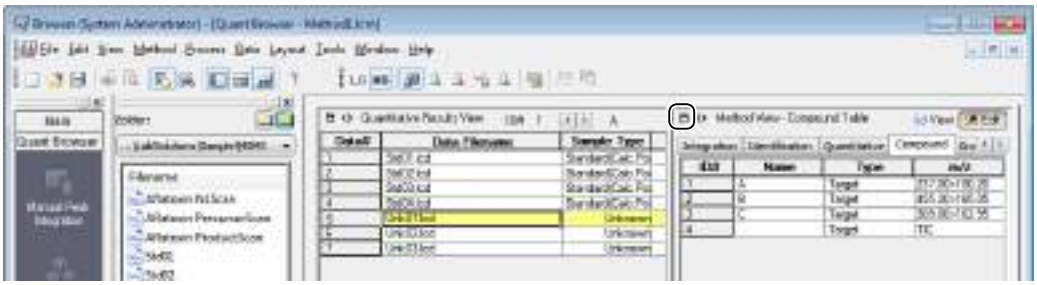
## 11.3.1 Edit the Compound Table

Compound Tables that were used for data acquisition can be edited in [Method View].

This section describes how to change [Conc. (1)] in the Compound Table.

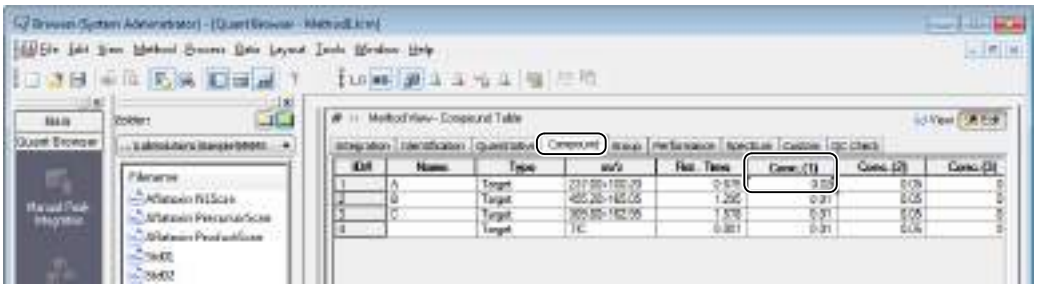
**1** **Click** Edit **(Edit Mode) in [Method View].**

## 2 Click (Full Size) in [Method View].

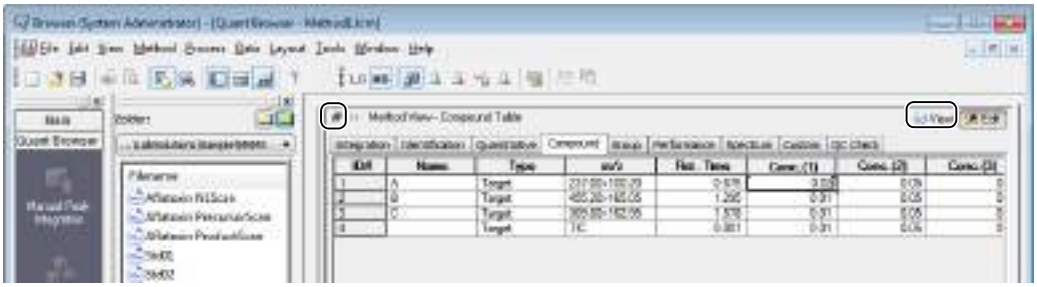


## 3 Click the [Compound] tab, select the desired compound, and change [Conc. (1)].

In this example, change the [Conc. (1)] setting from “0.01” to “0.02”.

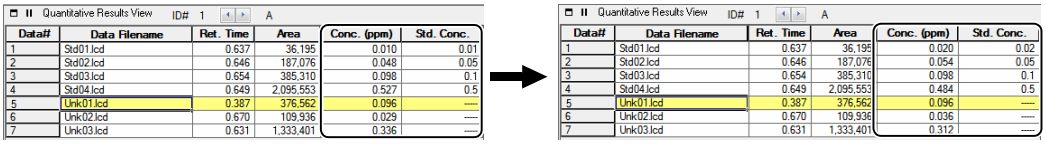


## 4 Click (Normal Size) and View (View Mode) in [Method View].



## 5 Click the (Peak Integration for All Data) icon on the [Quant Browser] assistant bar, and then click [OK].

The calibration curve is recreated, the quantitative results are re-calculated, and [Quantitative Results View] is updated.



Quantitative Results View ID# 1 A

| Data# | Data Filename | Ret. Time | Area | Conc. (ppm) | Std. Conc. |
|---|---|---|---|---|---|
| 1 | Std01.lcd | 0.637 | 36,195 | 0.010 | 0.01 |
| 2 | Std02.lcd | 0.646 | 187,076 | 0.048 | 0.05 |
| 3 | Std03.lcd | 0.654 | 385,310 | 0.098 | 0.1 |
| 4 | Std04.lcd | 0.649 | 2,095,553 | 0.527 | 0.5 |
| 5 | Unk01.lcd | 0.387 | 376,562 | 0.096 | ---- |
| 6 | Unk02.lcd | 0.670 | 109,936 | 0.029 | ---- |
| 7 | Unk03.lcd | 0.631 | 1,333,401 | 0.336 | ---- |

Quantitative Results View ID# 1 A

| Data# | Data Filename | Ret. Time | Area | Conc. (ppm) | Std. Conc. |
|---|---|---|---|---|---|
| 1 | Std01.lcd | 0.637 | 36,195 | 0.020 | 0.02 |
| 2 | Std02.lcd | 0.646 | 187,076 | 0.054 | 0.05 |
| 3 | Std03.lcd | 0.654 | 385,310 | 0.098 | 0.1 |
| 4 | Std04.lcd | 0.649 | 2,095,553 | 0.484 | 0.5 |
| 5 | Unk01.lcd | 0.387 | 376,562 | 0.096 | ---- |
| 6 | Unk02.lcd | 0.670 | 109,936 | 0.036 | ---- |
| 7 | Unk03.lcd | 0.631 | 1,333,401 | 0.312 | ---- |

**NOTE**

- Right-click on [Method View] and click [Cancel Edit] to cancel method editing.
- Select the columns that are displayed in the Compound Table in the [Table Style] sub-window. Right-click on the Compound Table and click [Table Style] to open the [Table Style] sub-window.

## 11.3.2 Edit [Quantitative Results View]

This section describes how to change the items displayed in the [Quantitative Results View].

Quantitative results are automatically re-calculated when each item is changed.

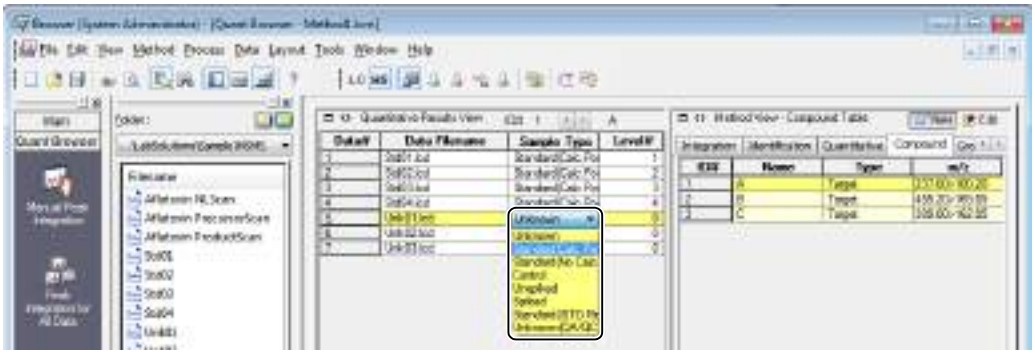
**NOTE**

- Right-click on [Quantitative Results View] and click [Remove] to delete a data file in [Quantitative Results View]. If deletion of a data file affects the calibration curve, all data files are re-calculated.
- Click the  icon on the toolbar to filter the data files displayed in [Quantitative Results View] by individual sample type.
- Right-click on [Quantitative Results View] and click [Full Path] to display the folder and file name at [Data Filename].
- Click the title of a column in the [Quantitative Results View] table to sort the data by [Data Filename], [Sample Name], [Sample ID], [Sample Type], [Level #], [Vial #], [Tray], and [Date Acquired].
  - Select the columns that are displayed in the [Quantitative Results View] table in the [Table Style] sub-window. Right-click on the [Quantitative Results View] table and click [Table Style] to open the [Table Style] sub-window.
- Click [Save Method File] on the [File] menu to save changes made to the data and method files in [Quantitative Results View].

## ■ Change the Sample Type

Sample types that were set at data acquisition can be changed.

**1** **Click the [Sample Type] cell of the sample to be changed, and select the sample type from the displayed list.**



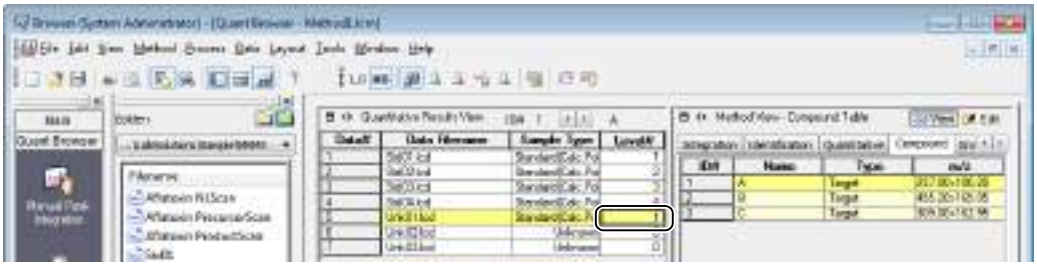
**NOTE**

If [Standard (Calc. Point)] is changed to another sample type, or another sample type is changed to [Standard (Calc. Point)], the calibration curve is re-created, and all data files are re-calculated.

## ■ Change the [Level#]

The level numbers that were set at data acquisition can be changed.

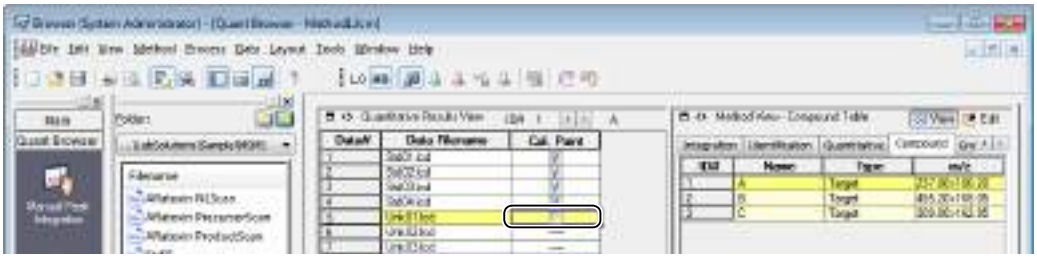
**1** **Change the [Level#] of the desired sample.**



## ■ Disable Calibration Points

Calibration curve points can be disabled if the standard samples were not analyzed appropriately.

**1** **Deselect [Cal. Point].**



If a [Cal. Point] is disabled, the calibration curve is re-created.

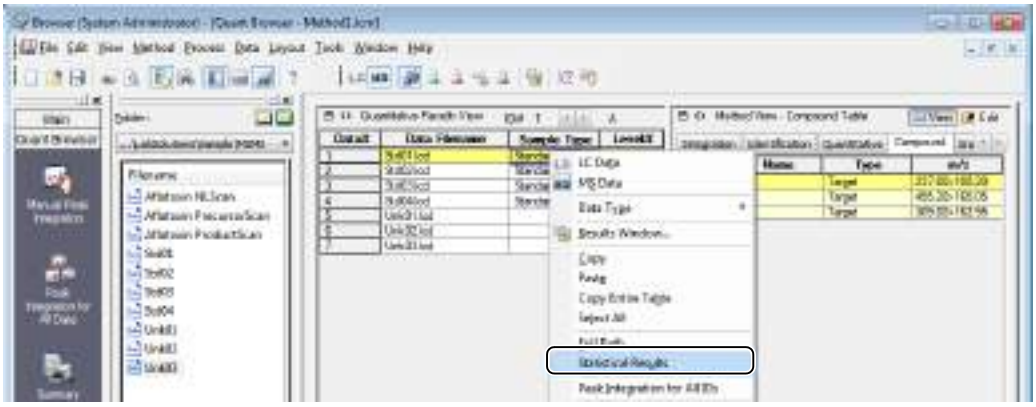
**NOTE**

Calibration points for individual compounds can be enabled or disabled on the [Compound] tab in [Method View].

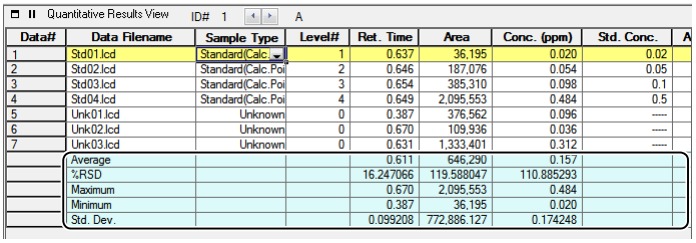
## ■ Display Statistical Results

Statistical calculations can be applied to quantitative results and the results can be displayed in the [Quantitative Results View].

**1** **Right-click on [Quantitative Results View], and click [Statistical Result].**



The statistical calculation results are added to the bottom of the table.



| Data# | Data Filename | Sample Type | Level# | Ret. Time | Area | Conc. (ppm) | Std. Conc. |
|---|---|---|---|---|---|---|---|
| 1 | Std01.lcd | Standard(Calc | 1 | 0.637 | 36,195 | 0.020 | 0.02 |
| 2 | Std02.lcd | Standard(Calc.Poi | 2 | 0.646 | 187,076 | 0.054 | 0.05 |
| 3 | Std03.lcd | Standard(Calc.Poi | 3 | 0.654 | 385,310 | 0.098 | 0.1 |
| 4 | Std04.lcd | Standard(Calc.Poi | 4 | 0.649 | 2,095,553 | 0.484 | 0.5 |
| 5 | Unk01.lcd | Unknown | 0 | 0.387 | 376,562 | 0.096 | ----- |
| 6 | Unk02.lcd | Unknown | 0 | 0.670 | 109,936 | 0.036 | ----- |
| 7 | Unk03.lcd | Unknown | 0 | 0.631 | 1,333,401 | 0.312 | ----- |
| | Average | | | 0.611 | 646,290 | 0.157 | |
| | %RSD | | | 16.247066 | 119.588047 | 110.885293 | |
| | Maximum | | | 0.670 | 2,095,553 | 0.484 | |
| | Minimum | | | 0.387 | 36,195 | 0.020 | |
| | Std. Dev. | | | 0.099208 | 772,886.127 | 0.174248 | |

**NOTE**

Select the [Statistic] column in the [Quantitative Results View] table to target a data file for statistical calculation. [Statistic] is not displayed in [Quantitative Results View] by default. Right-click on the [Quantitative Results View] table and select [Table Style] to display the [Statistic] column.

# 11.3.3 Change Peak Integration Parameters

This section describes how to change the peak integration parameters and re-integrate the peak.

**1** **Click Edit (Edit Mode) in [Method View].**

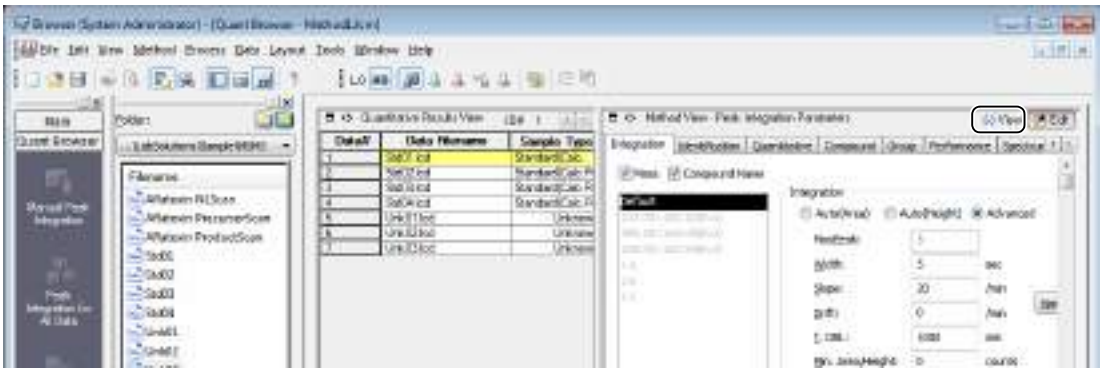
## 2 Click the [Integration] tab, and set each parameter as required.

In this example, change the [Slope] to “20”.

**Reference**

Refer to the Data Acquisition & Processing Theory Guide for details on peak integration.

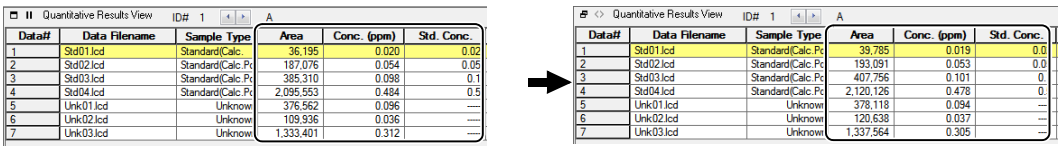
## 3 Click View (View Mode) in [Method View].



## 4 Select [Peak Integration] on the [Process] menu, and click [Peak Integration for All IDs of All Data].

[Peak Integration for All IDs of All Data] executes peak integration on all IDs of all currently loaded data files.

The results of peak integration and quantitation are displayed in the [Quantitative Results View].



Quantitative Results View ID# 1 A

| Data# | Data Filename | Sample Type | Area | Conc. (ppm) | Std. Conc. |
|---|---|---|---|---|---|
| 1 | Std01.lcd | Standard(Calc. | 36,195 | 0.020 | 0.02 |
| 2 | Std02.lcd | Standard(Calc.Pc | 187,076 | 0.054 | 0.05 |
| 3 | Std03.lcd | Standard(Calc.Pc | 385,310 | 0.098 | 0.1 |
| 4 | Std04.lcd | Standard(Calc.Pc | 2,095,553 | 0.484 | 0.5 |
| 5 | Unk01.lcd | Unknow | 376,562 | 0.096 | --- |
| 6 | Unk02.lcd | Unknow | 109,936 | 0.036 | --- |
| 7 | Unk03.lcd | Unknow | 1,333,401 | 0.312 | --- |

Quantitative Results View ID# 1 A

| Data# | Data Filename | Sample Type | Area | Conc. (ppm) | Std. Conc. |
|---|---|---|---|---|---|
| 1 | Std01.lcd | Standard(Calc.Pc | 39,785 | 0.019 | 0.0 |
| 2 | Std02.lcd | Standard(Calc.Pc | 193,091 | 0.053 | 0.0 |
| 3 | Std03.lcd | Standard(Calc.Pc | 407,756 | 0.101 | 0. |
| 4 | Std04.lcd | Standard(Calc.Pc | 2,120,126 | 0.478 | 0. |
| 5 | Unk01.lcd | Unknow | 378,118 | 0.094 | --- |
| 6 | Unk02.lcd | Unknow | 120,638 | 0.037 | --- |
| 7 | Unk03.lcd | Unknow | 1,337,564 | 0.305 | --- |

**NOTE**

- Quantitation is performed following peak integration.
- Either click (Peak Integration (ID)) on the toolbar, or select [Peak Integration] on the [Process] menu, and click [Peak Integration by ID] to perform peak integration on the displayed IDs for the selected data files.
- Select [Peak Integration] on the [Process] menu and click [Peak Integration for all IDs] to perform peak integration on all IDs for the selected data files.

## 11.3.4 Calibration Curve Correction

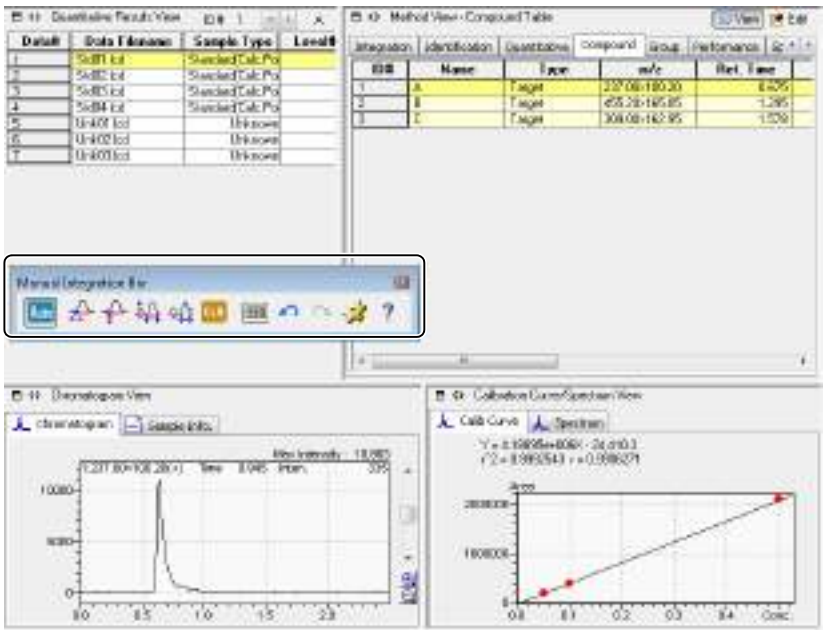
During calibration curve creation, low-concentration samples may not be integrated properly. If the low-concentration calibration point is disabled, a 3-point calibration curve becomes a 2-point calibration curve.

This section describes how to manually integrate the data of a standard sample that could not be automatically integrated, and correct the calibration curve.

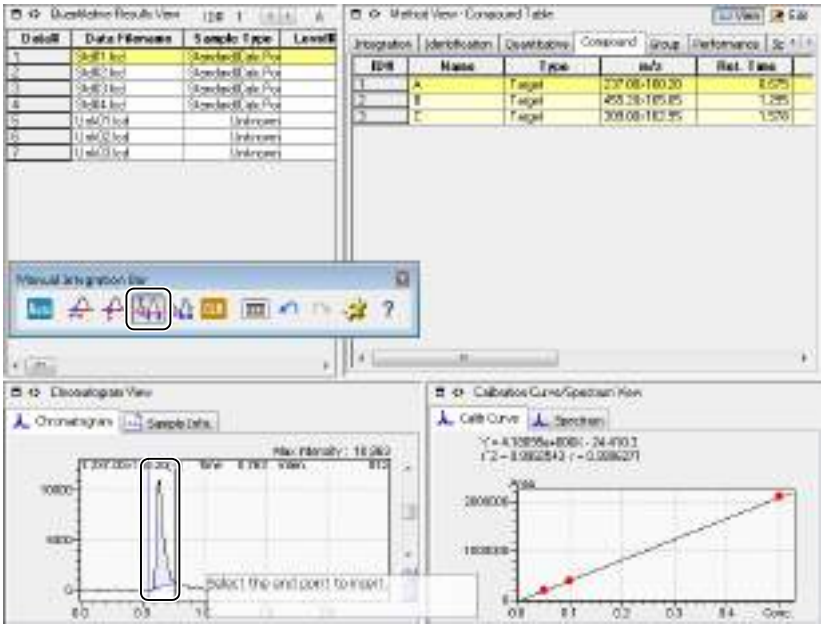
This section describes an example where peak integration failed, resulting in 2-point calibration curve.

**1 Click the (Manual Peak Integration) icon on the [Quant Browser] assistant bar in the [Browser] program.**

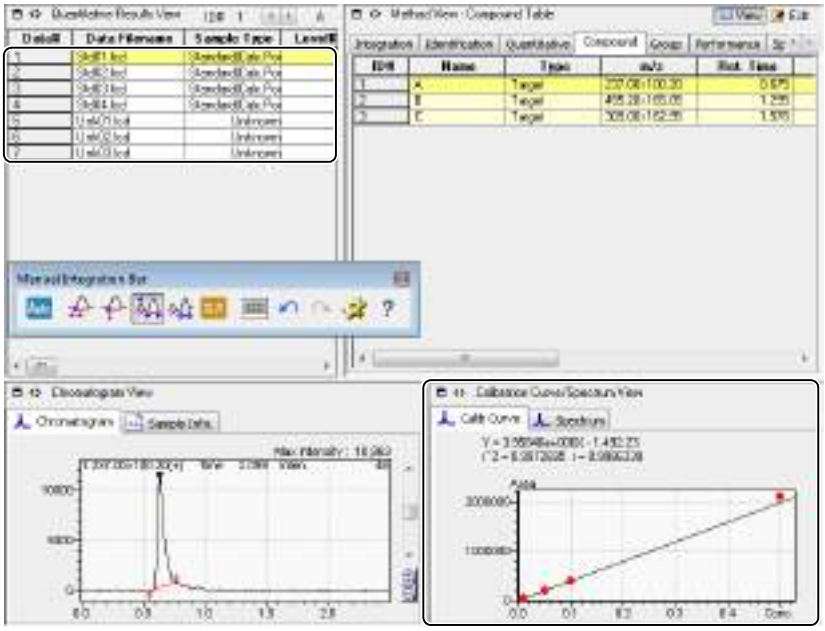
The [Manual Integration Bar] is displayed.



## 2 Click (Clear & Insert Peak) on [Manual Integration Bar], and click the peak start point and then the peak end point.



The peak is detected, and the results are re-calculated.
The 4-point calibration curve is re-created, and all data files are recalculated.



**NOTE**

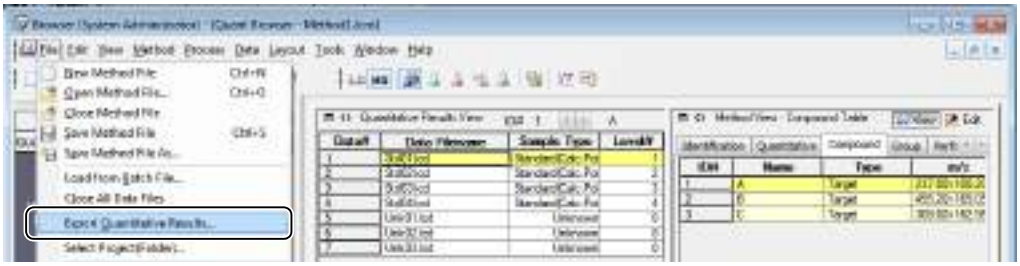
To confirm the calibration curve information, right-click on the calibration curve on the [Calib Curve] tab in [Calibration Curve/Spectrum View], and click [Calibration Information] on the displayed menu.

Peaks can be inserted by using Auto (Auto Mode) or (Clear & Insert Peak) icon.

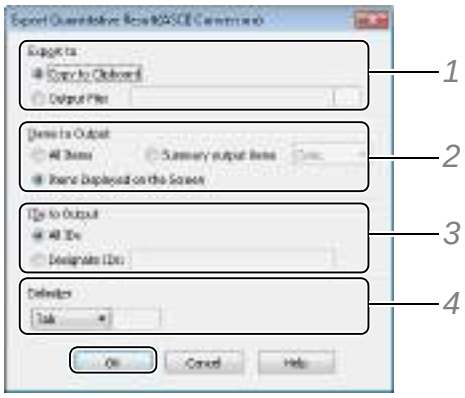
## 11.3.5 Export the Quantitative Results

The contents of the [Quantitative Results View] table can be converted to the ASCII text format and saved to a file or copied to the Clipboard.

**1** **Click [Export Quantitative Results] on the [File] menu.**



**2** **Select the desired parameters, and click [OK].**




*1* Select [Export to].

Enter the folder and file name to output files.

*2* Set [Items to Output].

Select [Items Displayed on the Screen] to output the items displayed in the [Quantitative Results View].

*3* Set [IDs to Output].

Select [All IDs] to display the results of all compound IDs.

Select [Designate IDs] and enter the ID numbers of the compounds to output.

- Enter multiple ID numbers to output with a comma or space. (example: 1,3,8)
- Enter a range of continuous ID numbers with a hyphen. (example: 2-8)

*4* Select a [Delimiter].

# 11.4 Print Quantitative Results

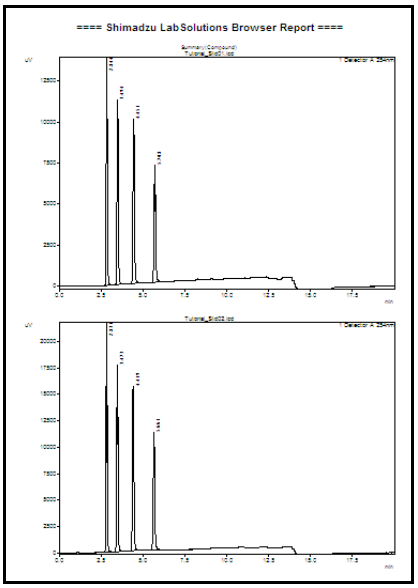
The [Quant Browser] window has a summary report function for collectively reporting multiple data.

**1** **Click the (Summary Report) icon on the [Quant Browser] assistant bar.**

**2** **Click the (Print) icon on the [Report] assistant bar.**

An image of the table is printed for each compound.

### Example of Quant Browser printout



# 12 Data Browser

Use the [Data Browser] window to compare multiple data, compare the data of different detectors, set the layout of display data, perform peak integration of chromatograms, and print browser reports.

This chapter describes how to collectively check multiple chromatograms and spectra.

## 12.1 Open the [Data Browser] Window

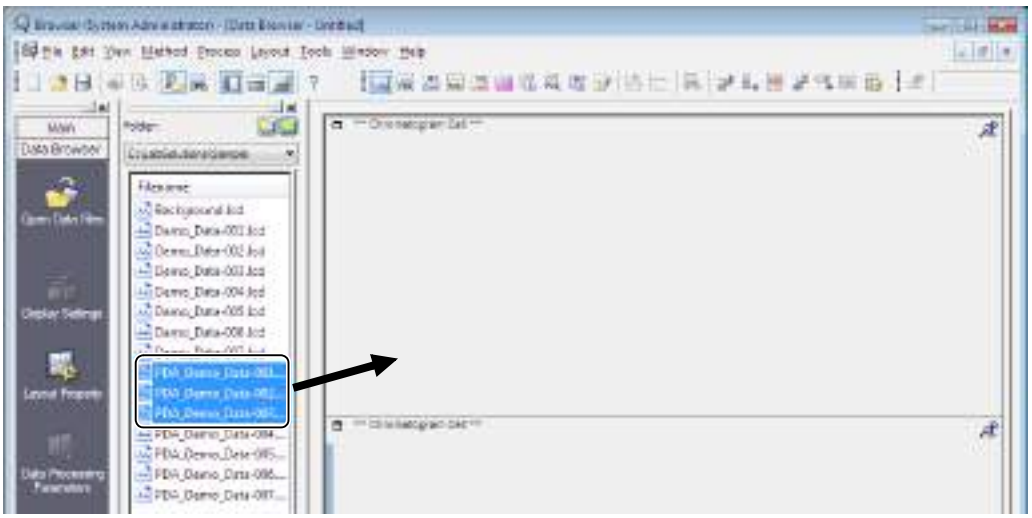
Up to 64 chromatogram data, sample information, etc. can be displayed as a list in the [Data Browser] Window.

**1 Select the  icon on the [LabSolutions Main] icon bar, and double-click the  icon.**

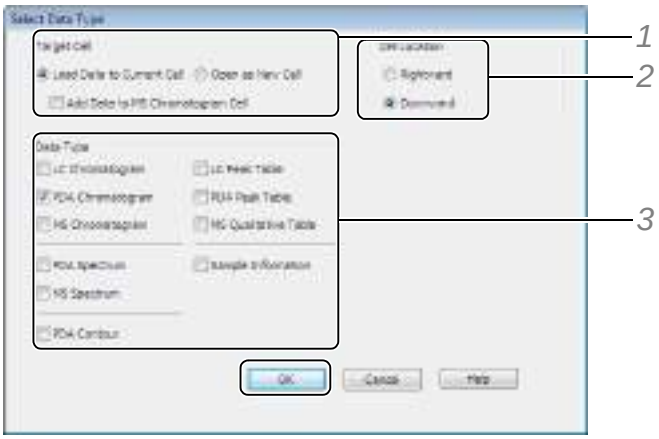
The [Browser] program opens.

**2** **Click the (Data Browser) icon on the [Main] assistant bar in the [Browser] program.**

**3** **Drag-and-drop the data files onto the [Data Browser] window from the [Data Explorer] sub-window.**



**4** **Select the Data Type parameters, and click [OK].**




**NOTE**

- If the cell fixed function is not enabled, the [Select Data Type] sub-window is displayed. Refer to *"12.3 Cell Fixed Function" P.358* for details on the cell fixed function.
- Multiple chromatogram data can be opened in a single cell to be displayed as an overlaid or stacked chromatogram.

1 Select the [Target Cell].

Select [Load Data to Current Cell] to display the selected data files in the cell where the files were dragged-and-dropped into from the [Data Explorer] sub-window.

Select [Add data to MS Chromatogram] to display chromatograms of different data files in the same cell.

Select [Open as New Cell] to display each data file in a new cell. Determine which direction to open the new cell in at [Cell Location].

**NOTE**

[Add data to MS Chromatogram] is only available when data files are dragged-and-dropped into an [MS Chromatogram] cell. Select from three types of chromatograms, [Chromatogram], [PDA Chromatogram] or [MS Chromatogram] at [Data Type], and chromatograms are displayed in the [MS Chromatogram] cell.

2 Set [Cell Location].

If [Open as New Cell] was selected at [Target Cell], set the direction that new cells will be added. Select [Rightward] to create columns and select [Downward] to create rows.

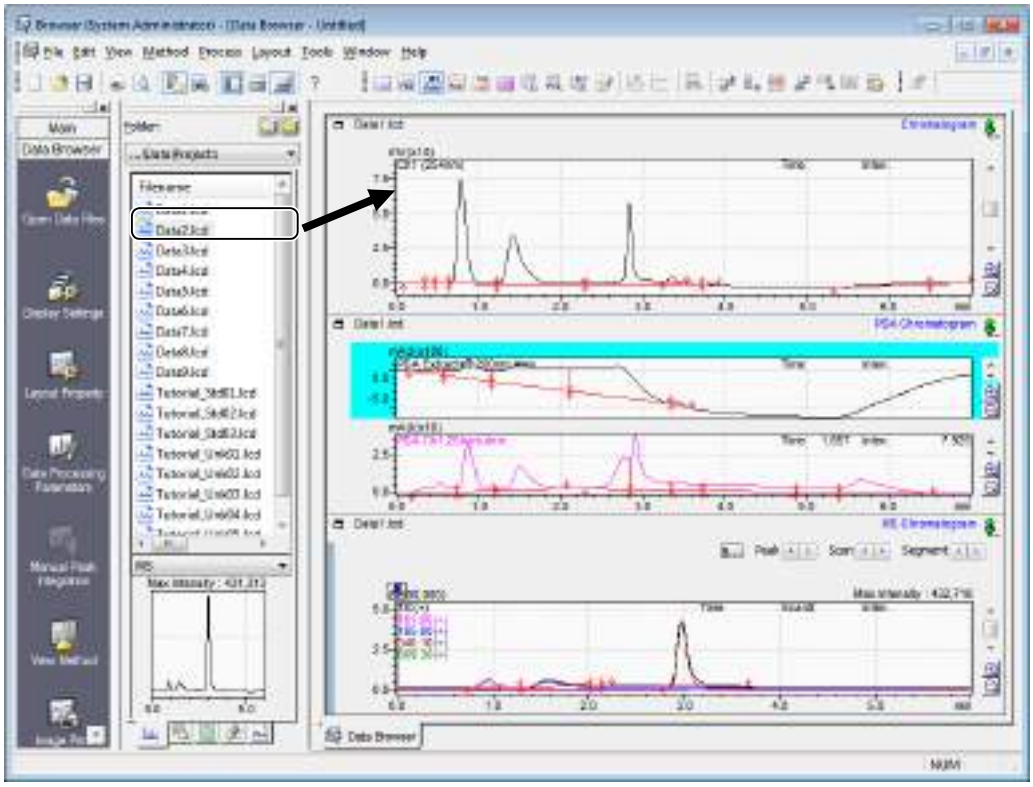
3 Set [Data Type].

Select the multiple types of data to be displayed.

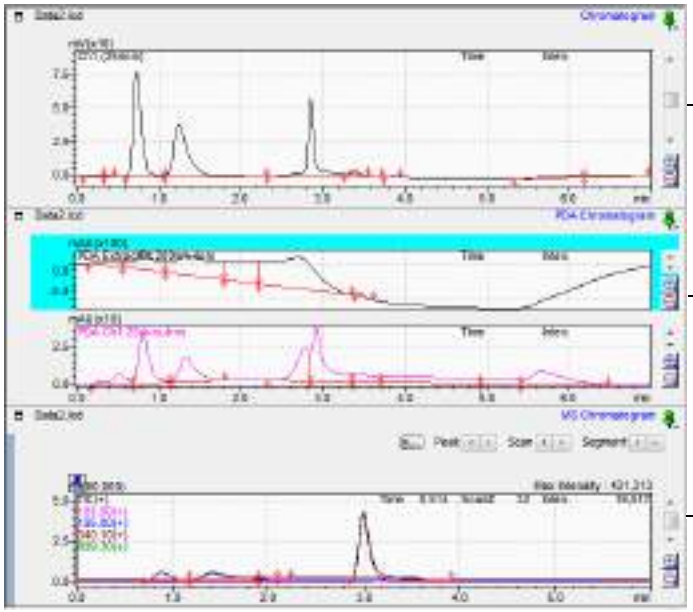
The contents of the data files are displayed in the [Data Browser] window.

## ■ [Target Cell]

Cells are created according to the [Target Cell] setting in the [Select Data Type] sub-window. The following example assumes that a data file is already loaded in a layout whose [Row] and [Col] settings are set to “3” and “1”, respectively.



- **[Load Data to Current Cell] is selected at [Target Cell] and [Add data to MS Chromatogram] is not selected**
  The [MS Chromatogram] cell contents are replaced by the data file that is dragged-and-dropped into that cell. In this example, the cell contents are overwritten with the [Chromatogram] and the [PDA Chromatogram] and [MS Chromatogram] are opened in the direction specified at [Cell Location]. Here, the [PDA Chromatogram] cell and [MS Chromatogram] are overwritten to cells below the cell that the data file was dragged-and-dropped into.

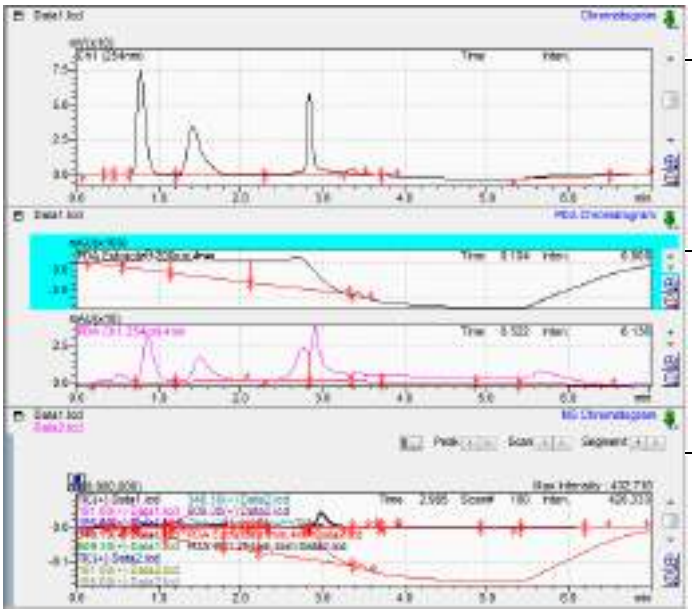



**NOTE**

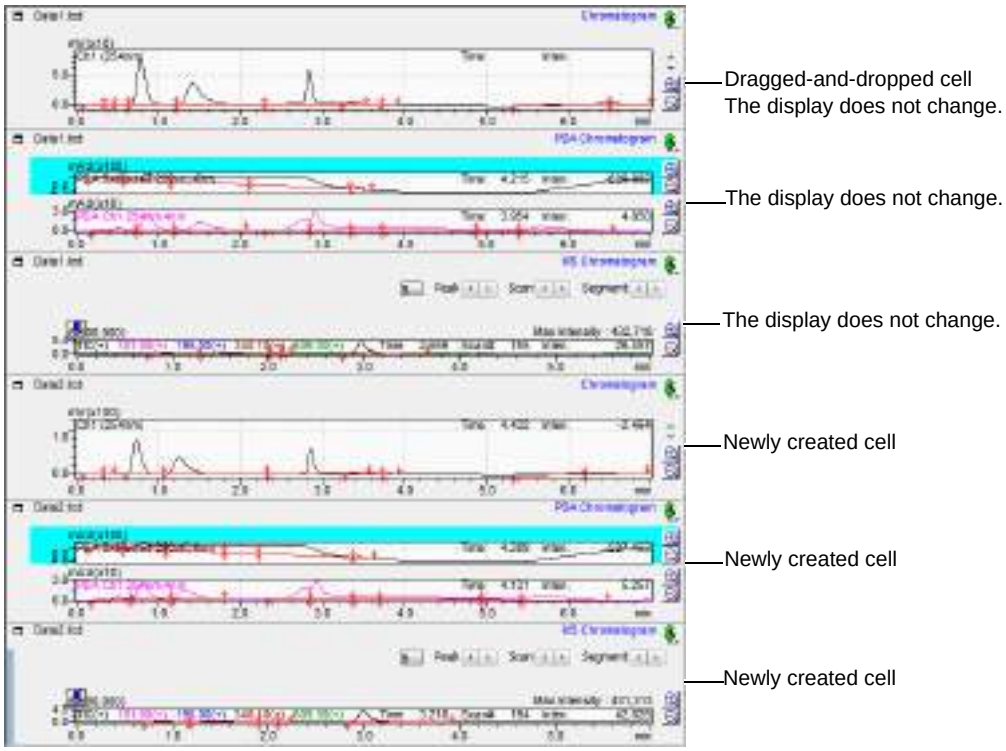
The cell order becomes [Chromatogram], [PDA Chromatogram] and [MS Chromatogram].

If multiple data files are dragged-and-dropped, only the data file initially selected in the [Data Explorer] sub-window is processed.

- **[Load Data to Current Cell] is selected and [Add data to MS Chromatogram] is selected)**
  The contents of the data files are added to and displayed in the [MS Chromatogram] cell into which the data file was dragged-and-dropped.



- **[Open as New Cell] is selected**
  New cells are created to individually display the [Chromatogram], [PDA Chromatogram] and [MS Chromatogram].

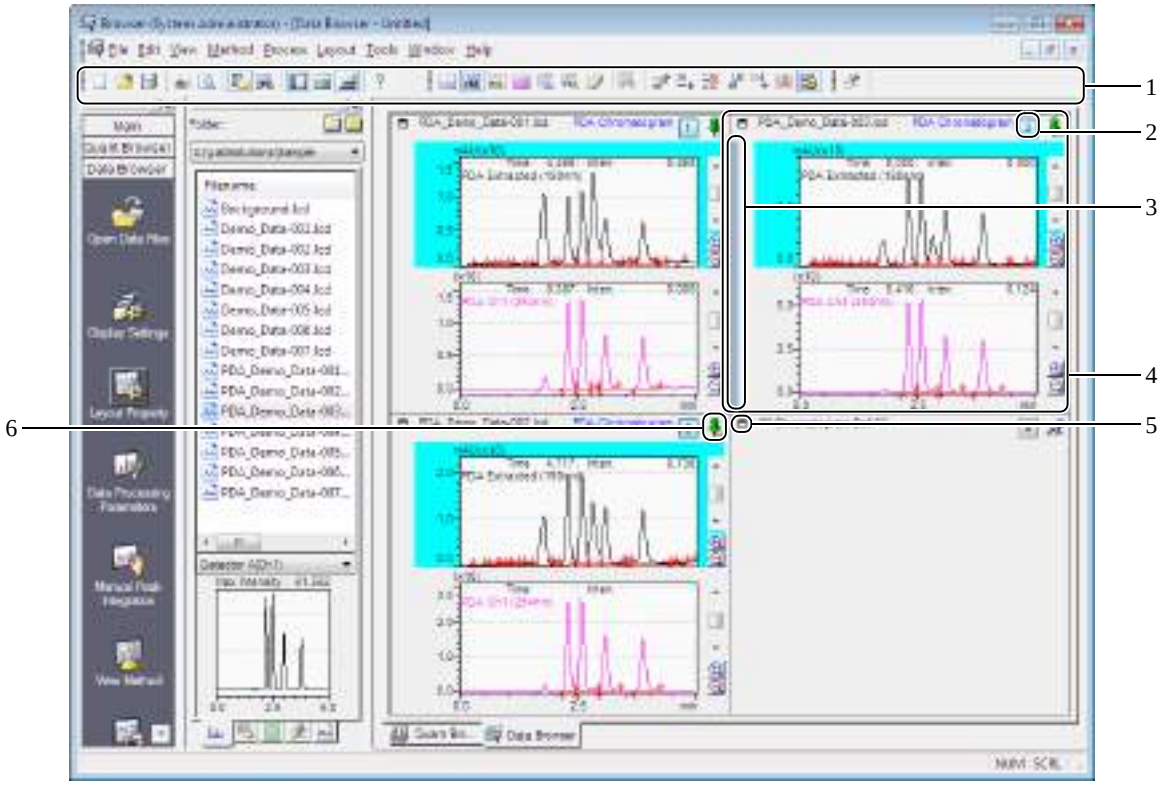



**NOTE**

If the [Row] or [Col] display reaches the maximum number of 8 each (8 rows, 8 columns), a new [Row] or [Col] is created to display the additional data files.

## 12.1.1 [Data Browser] Window Description

This section describes how to view and use the [Data Browser] window.




| No. | Explanation |
|---|---|
| 1 | Displays the [Standard] and [Data Browser] toolbars. |
| 2 | Displays the preset cell number. The cell number can be changed by clicking 1. If the cell fixed function is enabled, 1 is displayed. Refer to *"12.3 Cell Fixed Function" P.358* for details on the cell fixed function. |
| 3 | The focus bar is displayed in the currently selected cell. |
| 4 | Displays the content of the data file in the cell.<br>Place the mouse pointer over the data file name display area to display the sample information. |
| 5 | Clicking this button to expand the cell to the full screen view. |
| 6 | When the focus pin is upright and green ( ), it is linked to other cells.<br>Refer to *"12.4.7 Link Content Between Cells" P.372* for details on linking cells. |

**NOTE**

- Files currently being edited in other windows are [Read Only] and cannot be edited. Close the file in the other window and open the file again to edit these files.
- The arrangement of cells in the vertical direction is referred to as [Row], and the arrangement of cells in the horizontal direction is referred to as [Col].
- The maximum number of [Row] and [Col] is 8 each, which means that up to 64 cells can be displayed.

# 12.2 Adjust Layouts

Adjust and re-arrange layouts so that the content of the currently displayed data can be easily compared.

**NOTE**

- Drag the boarder of the [Data Browser] cell with the mouse to resize the cell. The size of [Data Browser] is automatically determined so that it is split into equal lengths according to the number of displayed cells.
- Use the cell connect function to partially create larger cells. Refer to *"12.2.3 Connect Cells" P.357* for details on connecting cells.

## 12.2.1 Adjust Display Layouts

This section describes how to adjust the layout of display cells.

**1** **Click the (Layout Property) icon on the [Data Browser] assistant bar.**

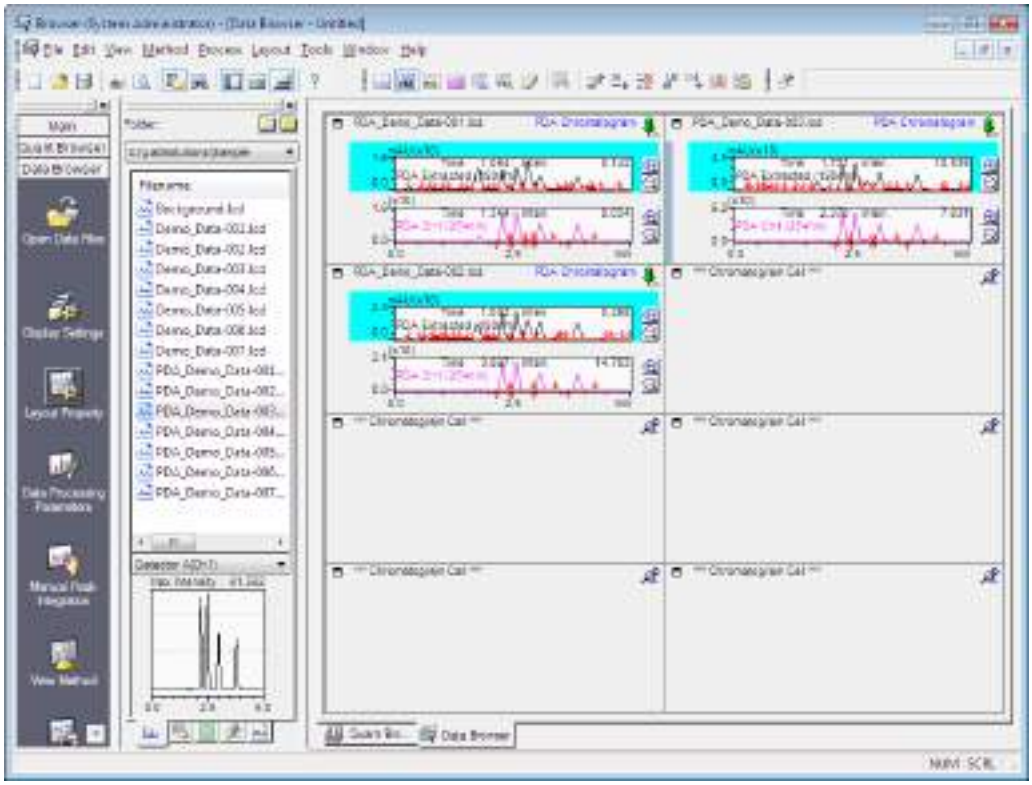
**NOTE**

The [Property] sub-window can also be opened by clicking [Property] on the [Layout] menu of the [Data Browser] window.

**2** **Select the [Style] tab, set the number of rows and columns of the cell to display, and click [OK].**

In this example, set [Row] and [Col] at [Cell Created] to “4” and “2”, respectively.

A 4 × 2 grid of cells is displayed.



**NOTE**

- Select [Scroll Mode] in the [Style] tab to display additional cells using the scroll bars. For example, when [Row] and [Col] at [Cell Displayed] are set to “3” and “2”, respectively, a 3 × 2 grid of cells is displayed in the sub-window and the remaining cells are displayed by scrolling with the scroll bars.
- To delete rows or columns, either right-click a cell in the row or column to be deleted, select [Adjust Layout], and click [Delete Row] or [Delete Column], or click (Delete Row) or (Delete Column) on the toolbar. Select the cell and click [Delete Cell] from the [Edit] menu to delete a single cell.
- Select [Save Layout File As] on the [Layout] menu to save cell layouts or the display information of data loaded to each cell. This data can be saved as layout files (file extension *.lyt).

## 12.2.2 Change the Contents of Cells

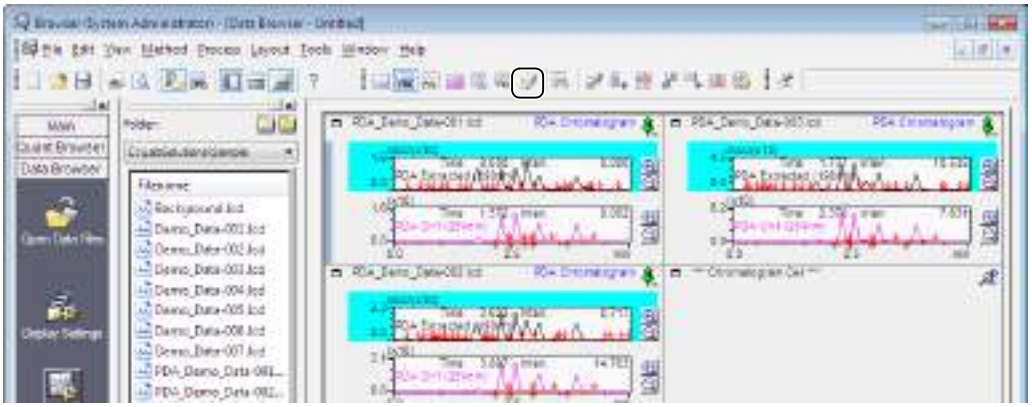
The contents displayed in cells in the [Data Browser] window can be changed.

This section describes how to change the cell content from [Chromatogram] to [Sample Information].

**1** **Click the desired cell.**

The focus bar is displayed.

**2** **Click (Sample Information) on the toolbar.**



**NOTE**

The display data can also be changed by right-clicking on the cell, selecting [Change Data Type], and clicking [Sample Information].

The display content of the cell is switched from a chromatogram to the sample information.

**NOTE**

- Click the  (Display Settings) icon on the [Data Browser] assistant bar to set the display mode and range of each cell. Refer to *"12.4.2 Change the Chromatogram Display Mode" P.361* for details on the display mode.
- Right-click on the source cell and click [Copy Cell] then right-click on the destination cell and click [Paste Cell] to copy the contents to other cells. This function is handy for displaying the contents of the same data file in multiple cells.
- To swap the contents of the currently selected cell with the contents of another cell, drag the title (file name) of the selected cell and drop it on the target cell.
- Right-click on the desired cell and click [Release Data from Cell] to delete the display contents of a cell.

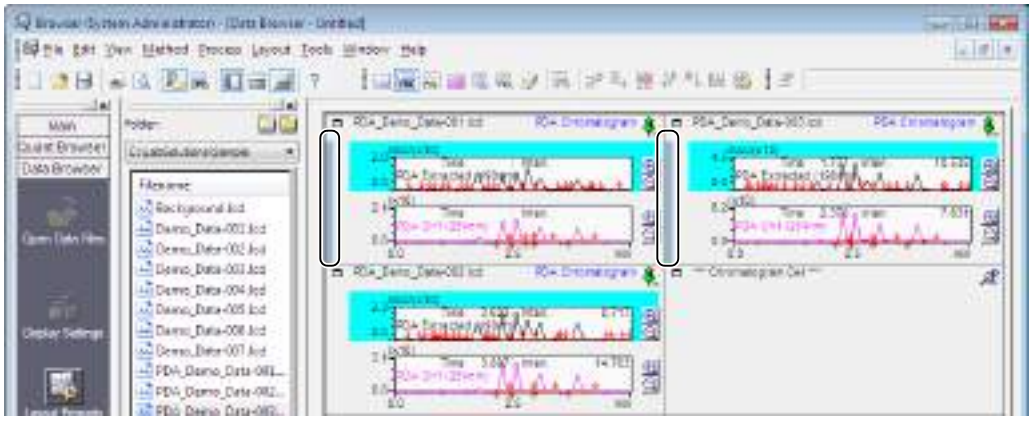
## 12.2.3 Connect Cells

Adjacent cells can be connected or disconnected.

This section describes how to connect cells.

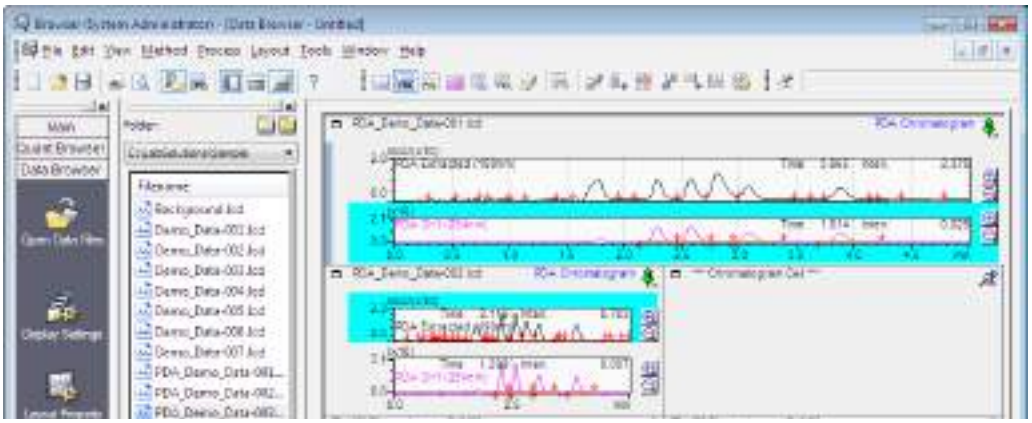
**1** **Select the cells to connect with the [Ctrl] key held down.**

The focus bar is displayed on the multiple cells.



**2** **Right-click on one of the selected cells and click [Connect Cell].**

The cells are connected.



**NOTE**

- When cells are connected, data which is open in secondary cells is closed.
- Right-click on the connected cell and click [Disconnect Cell] to disconnect cell connections.
- Select cells to be connected so that the shape of the resulting cell is a rectangle.

# 12.3 Cell Fixed Function

Use the cell fixed function to efficiently compare different data files. For example, compare the peaks of the control sample and target sample.

When the cell fixed function is used, the cell numbers are displayed in each cell. The contents of the same data file is displayed in cells of the same cell number.

**Reference**

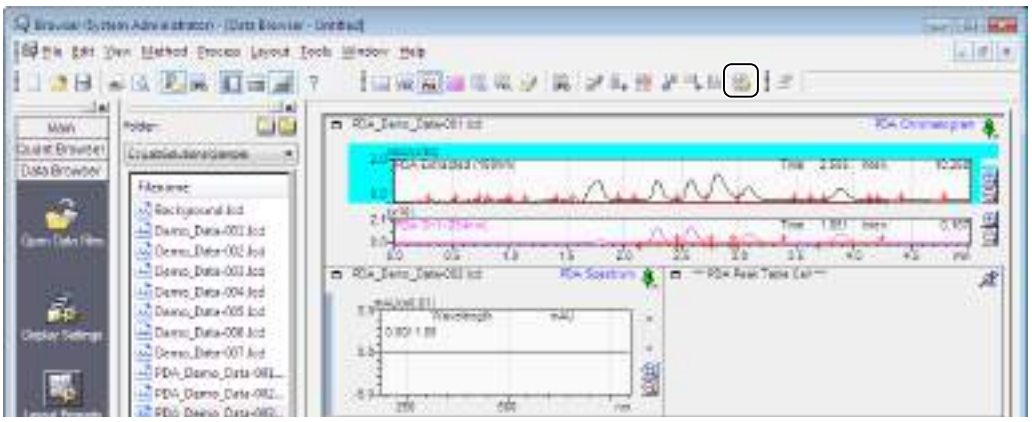
*"12.4.6 Load a Data File in Multiple Cells" P.368*

*"12.4.8 Peak Integration on Chromatograms" P.374*

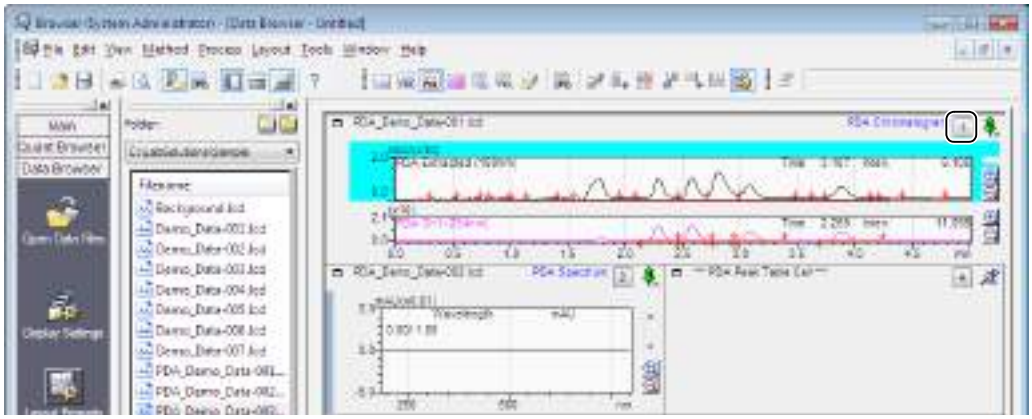
## 12.3.1 Use the Cell Fixed Function

This section describes how to turn the cell fixed function on.

**1** **Click the (Cell Fixed) icon on the toolbar.**



(Cell Fixed) is selected, and cell number ( 1 ) is displayed in the cell.



**NOTE**

- Click the (Cell Fixed) icon on the toolbar again, to turn the cell fixed function off.
- The cell fixed function can also be switched on and off by clicking [Cell Fixed] on the [Edit] menu in the [Data Browser] window.

# 12.4 Compare Data

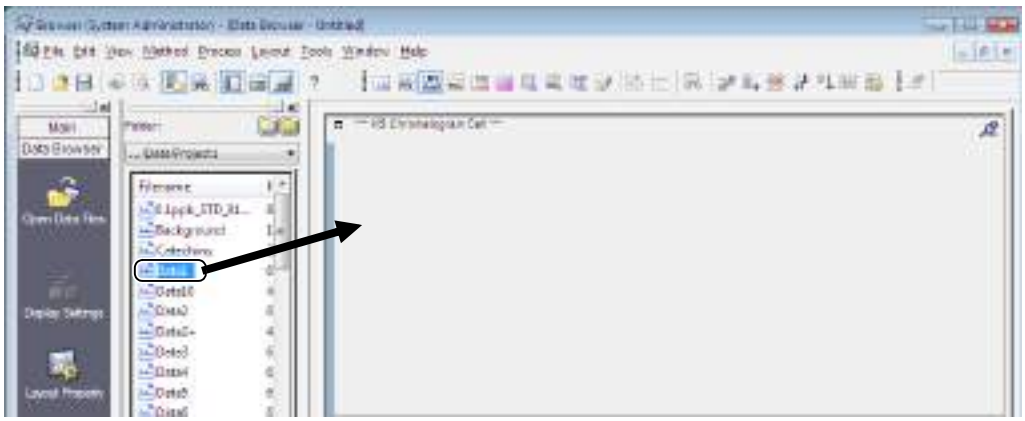
The chromatograms from different detectors or multiple data files can be displayed in the same [MS Chromatogram] cell. Data from different detectors can be overlaid.

## 12.4.1 Display the Chromatograms from Different Detectors in the Same Cell

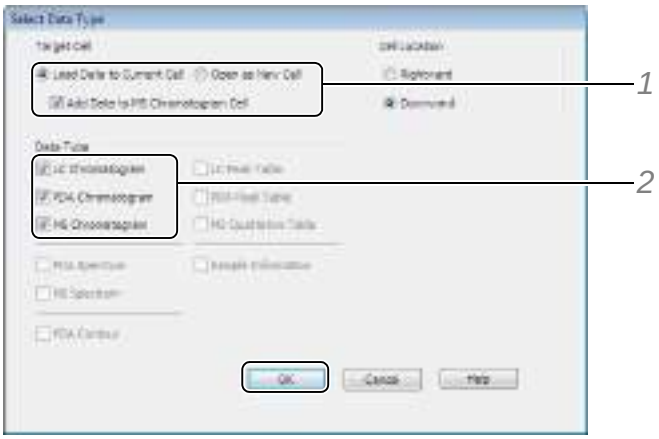
The chromatograms from different detectors can be displayed in the same [MS Chromatogram] cell.

This section describes how to display MS chromatograms, chromatograms and PDA chromatograms in the [MS Chromatogram] cell.

**1** **Drag-and-drop the data file onto the [MS Chromatogram] cell from the [Data Explorer] sub-window.**

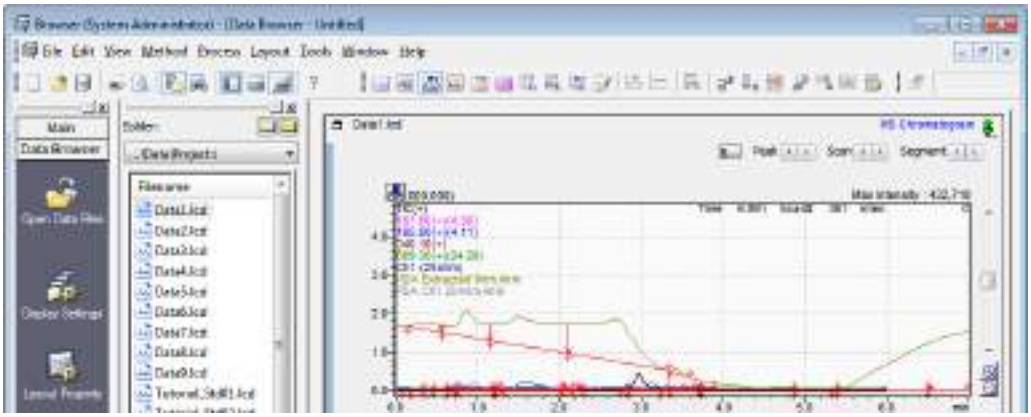


## 2 Set each item, and click [OK].




1 Select [Load Data to Current Cell], and select [Add data to MS Chromatogram].
2 Select [Chromatogram], [PDA Chromatogram] and [MS Chromatogram].

The [Chromatogram], [PDA Chromatogram] and [MS Chromatogram] are all displayed in the same cell.



## 12.4.2 Change the Chromatogram Display Mode

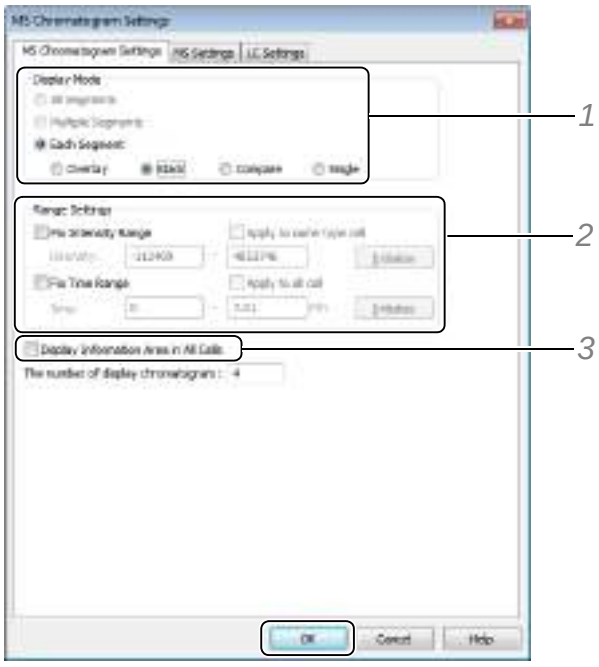
The chromatogram display mode in the [MS Chromatogram] can be changed to [All Segments], [Multiple Segments] or [Each Segment].

The [Overlay], [Stack], [Compare] and [Single] parameters are available for chromatograms in the [Each Segment] display mode.

This section describes how to change chromatogram display from [Overlay] to [Stack].

**1** **Select the [MS Chromatogram] cell to be changed, and click the  (Display Settings) icon on the [Data Browser] assistant bar.**

**2** **Click the [MS Chromatogram Settings] tab, set each item, and click [OK].**




*1* Set [Display Mode].
Select [Each Segment] and [Stack].

**Reference**

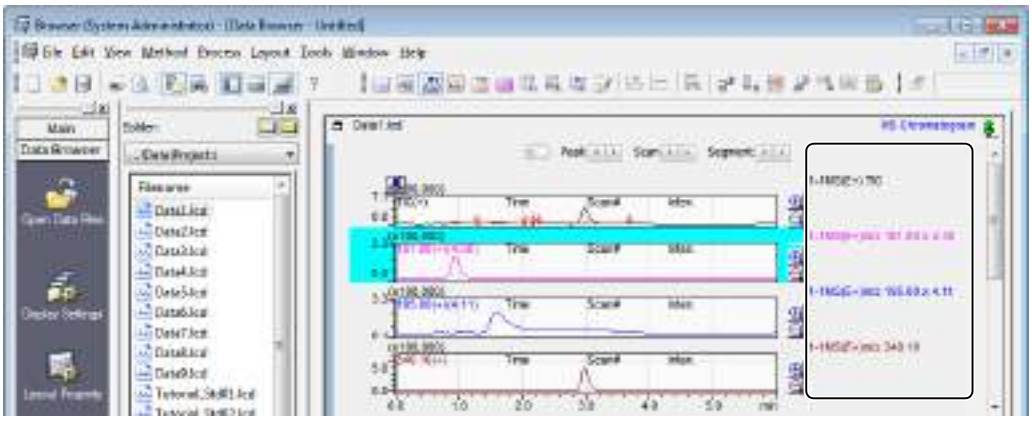
Refer to *"6.2.4 Change the [Chromatogram View] Display Mode" P.183* for details on [Display Mode].

2 Enter the [Range Settings].

The axis range can be fixed. Select [Apply to same type cell] or [Apply to all cell] to apply the same axis range to other cells. Click [Initialize] to return the range to its original setting.

3 Determine whether to display the information area in all of the cells.

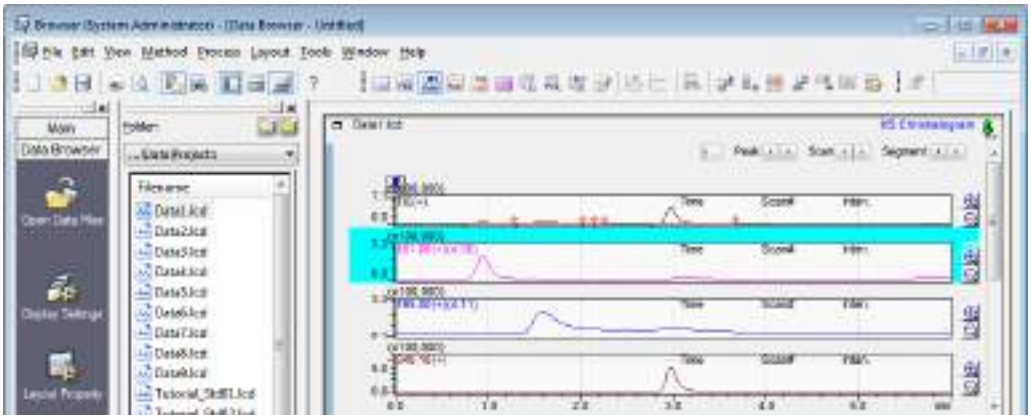
An information area is displayed on the right of all chromatogram and spectrum cells when [Display Information Area in All Cells] is selected.



**NOTE**

The [MS Chromatogram Settings] sub-window can also be displayed by right-clicking on the [MS Chromatogram] cell, and clicking [Display Settings].

[Display Mode] is changed to [Stack].



**NOTE**

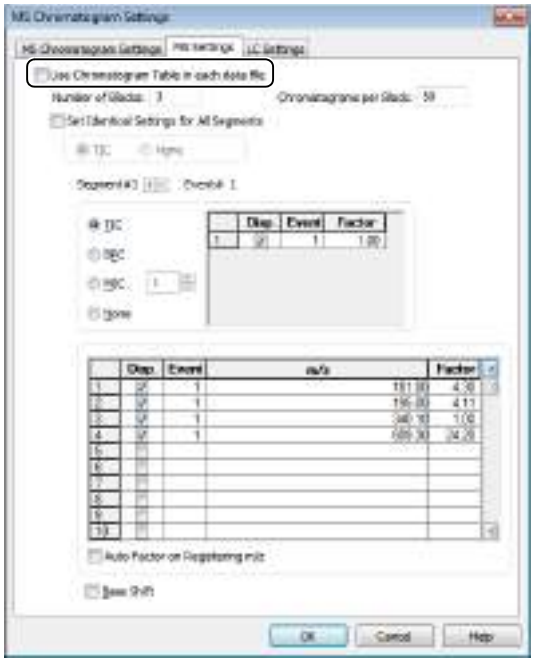
Up to 16 data files can be displayed in one [MS Chromatogram] cell.

## 12.4.3 Display or Hide the Chromatogram

Select or deselect [Disp.] on the [Chromatogram Table] tab or [LC Settings] tab in the [MS Chromatogram Settings] sub-window to display or hide chromatograms in the [MS Chromatogram] cell.

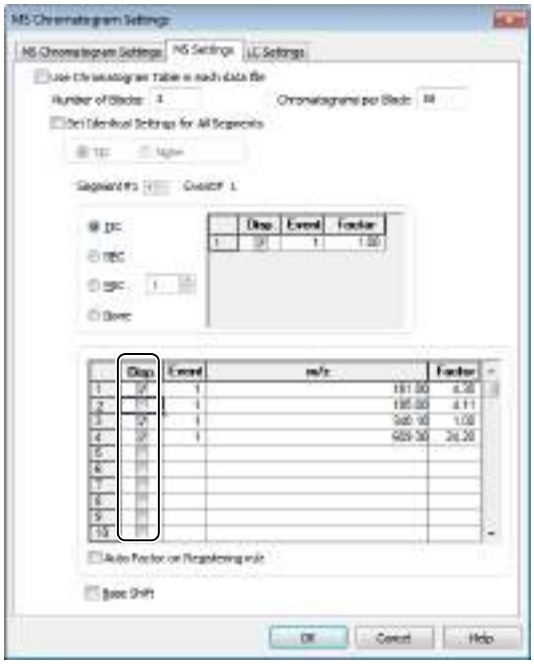
### ■ Hide Chromatograms in the [MS Chromatogram] Cell

**1** **Click the [MS Settings] tab in the [MS Chromatogram Settings] sub-window, and select [Use Chromatogram Table in each data file].**



**2** **Deselect the [Disp.] column for the MS chromatogram to be hidden in the Chromatogram Table, and click [OK].**

The [MS Chromatogram] cell is no longer displayed.



**NOTE**

When [Use Chromatogram Table in each data file] is selected, the chromatogram to display is based on the Chromatogram Table in the respective data file. When [Use Chromatogram Table in each data file] is not selected, the [MS Chromatogram Settings] can be applied to all open data in the [MS Chromatogram] cell.

**Reference**

Refer to *"6.2.6 Display Chromatograms from the Chromatogram Table and MIC Table" P.188* for details on the Chromatogram Table.

**3** **Click [Yes].**

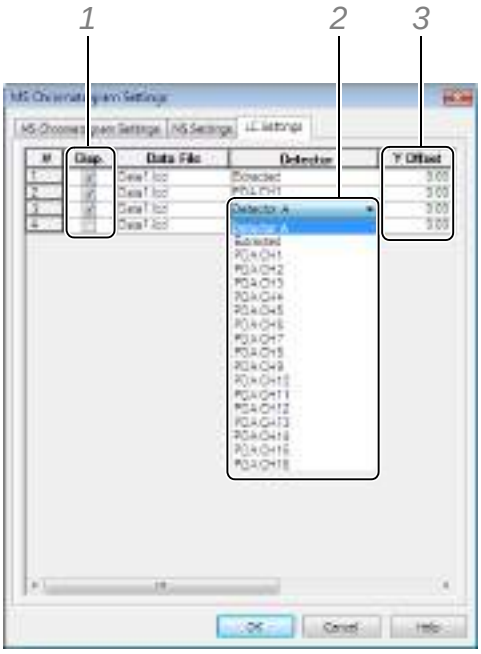
The settings are applied to all [MS Chromatogram] cell. Clicking [No], the settings are applied to the currently selected [MS Chromatogram] cell.


## ■ Hide Chromatograms and PDA Chromatograms

Chromatograms and PDA chromatograms displayed or hidden on the [LC Settings] tab in the [MS Chromatogram Settings] sub-window.

This section describes how to hide the [PDA Chromatogram].

**1** **Click the [LC Settings] tab in the [MS Chromatogram Settings] sub-window, set each item, and click [OK].**




*1* Deselect the [Disp.] column for the [PDA Chromatogram] cell to be hidden.

*2* Select the desired detector from the list of available detectors in the selected data file. Enter the amount of base shift for overlaid chromatograms.

3 Set the intensity axis scale for the chromatogram display.

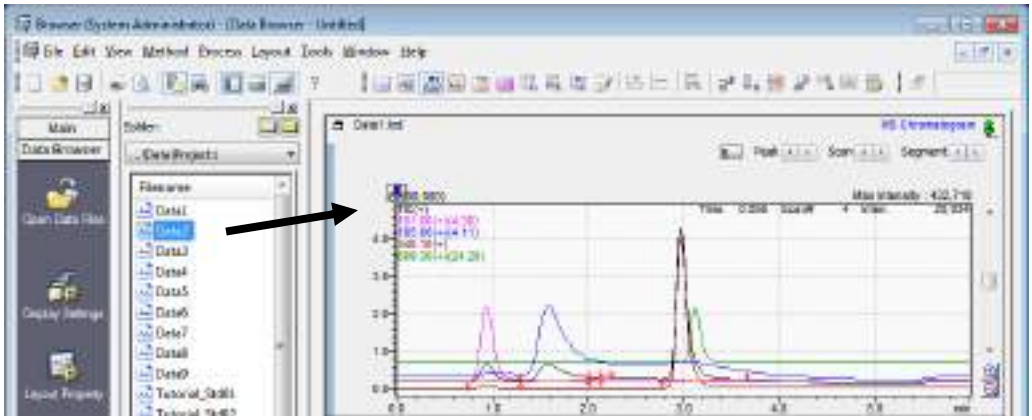
The [PDA Chromatogram] is no longer displayed.

## 12.4.4 Display Multiple Chromatograms in the Same Cell

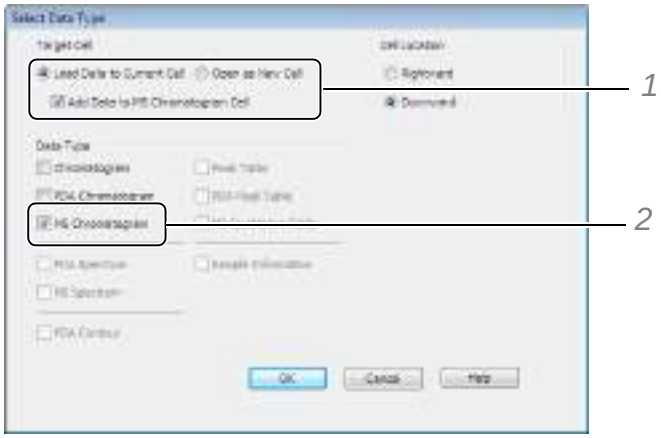
Multiple data file chromatograms can be displayed in the same [MS Chromatogram] cell.

In this example, the MS chromatogram of data file Data2.lcd is added to the [MS Chromatogram] cell that is currently displaying data file Data1.lcd.

**1 Drag-and-drop Data2.lcd onto the [MS Chromatogram] cell that is currently displaying Data1.lcd from the [Data Explorer] sub-window.**



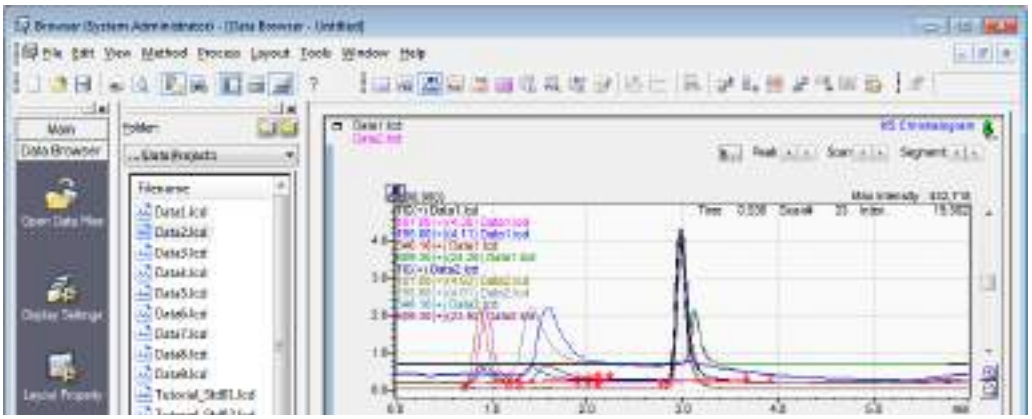
**2 Set each item, and click [OK].**




1 Select [Load Data to Current Cell] and [Add data to MS Chromatogram].

2 Select [MS Chromatogram] as the data type.

The MS chromatograms of Data1.lcd and Data2.lcd are displayed in the same cell.



**NOTE**

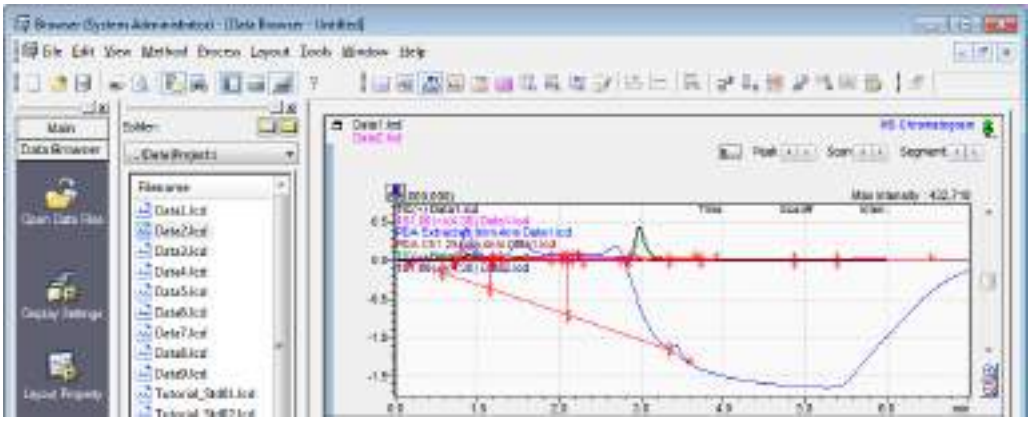
- The name of the data file highlighted at the top of the cell is the active data.
- Up to 80 chromatograms can be displayed in the same cell.

## 12.4.5 Time Compensation

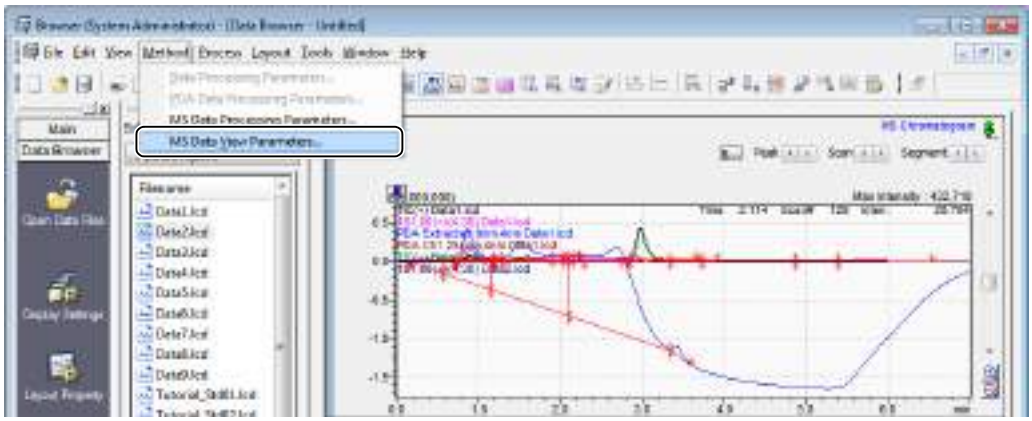
When the chromatograms of different detectors are displayed in the same cell, if there is a difference in the retention times, it is not always easy to determine whether the chromatograms are for the same substance. The time compensation function allows the chromatograms to be aligned by compensating for each detector.

This section describes how to align a [PDA Chromatogram] with the [MS Chromatogram].

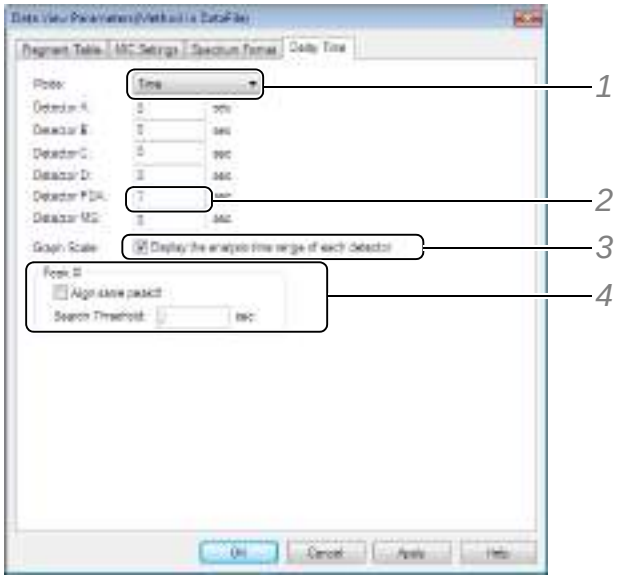
**1** **Display the chromatogram of the PDA detector in the [MS Chromatogram] cell.**



**2** **Click [MS Data View Parameters] on the [Method] menu.**




**3** **Click the [Delay Time] tab, set each item, and click [OK].**




1 Select whether to compensate by time or volume.

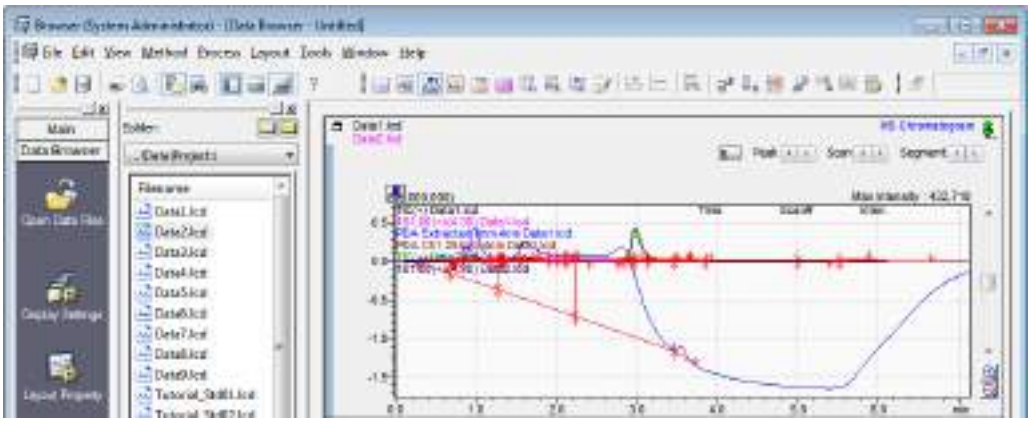
2 Set the compensation time or volume of each detector.

In this example, enter “7” sec. for the [Detector PDA].

3 If the [Display the analysis time range of each detector] checkbox is selected, the chromatogram is displayed in a time-compensated time range for each detector. If this checkbox is not selected, the chromatogram is displayed in a range that uses the minimum start time and maximum end time of all of the detectors.

4 When [Align same peak #] is selected, the same peak number can be assigned to peaks of each detector with the same retention time. Set the time width to be used for judgement of same peak at [Search Threshold].

The chromatograms are compensated.



## 12.4.6 Load a Data File in Multiple Cells

This section describes how to use the cell fixed function to display the chromatograms, PDA chromatograms and MS chromatograms of data files 1 and 2.

**1** **Determine the layout and cell type.**

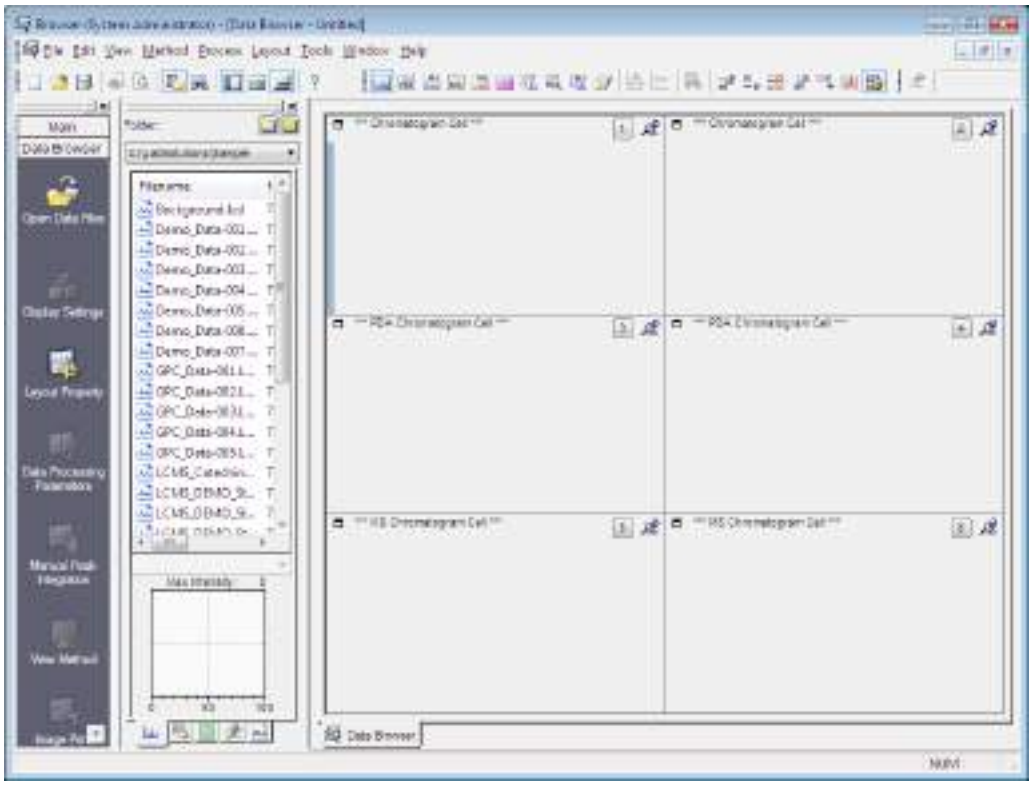
This example uses a 3 row × 2 column layout to display a chromatogram in the 1st row, a PDA chromatogram in the 2nd row, and an MS chromatogram in the 3rd row.

**Reference**

Refer to *"12.2.1 Adjust Display Layouts" P.354* for details on changing layouts, and *"12.2.2 Change the Contents of Cells" P.356* for changing cell type.

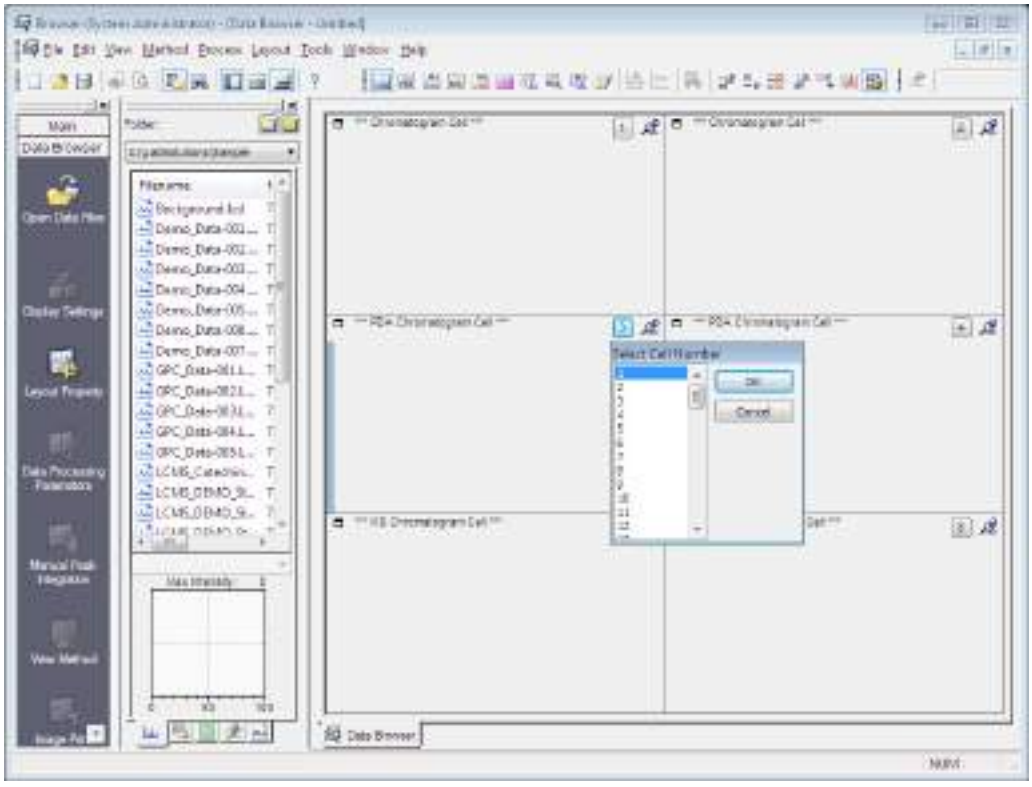
**2** **Click the (Cell Fixed) icon on the toolbar.**

(Cell Fixed) is selected and cell number ( 1 ) is displayed in the cell display area.

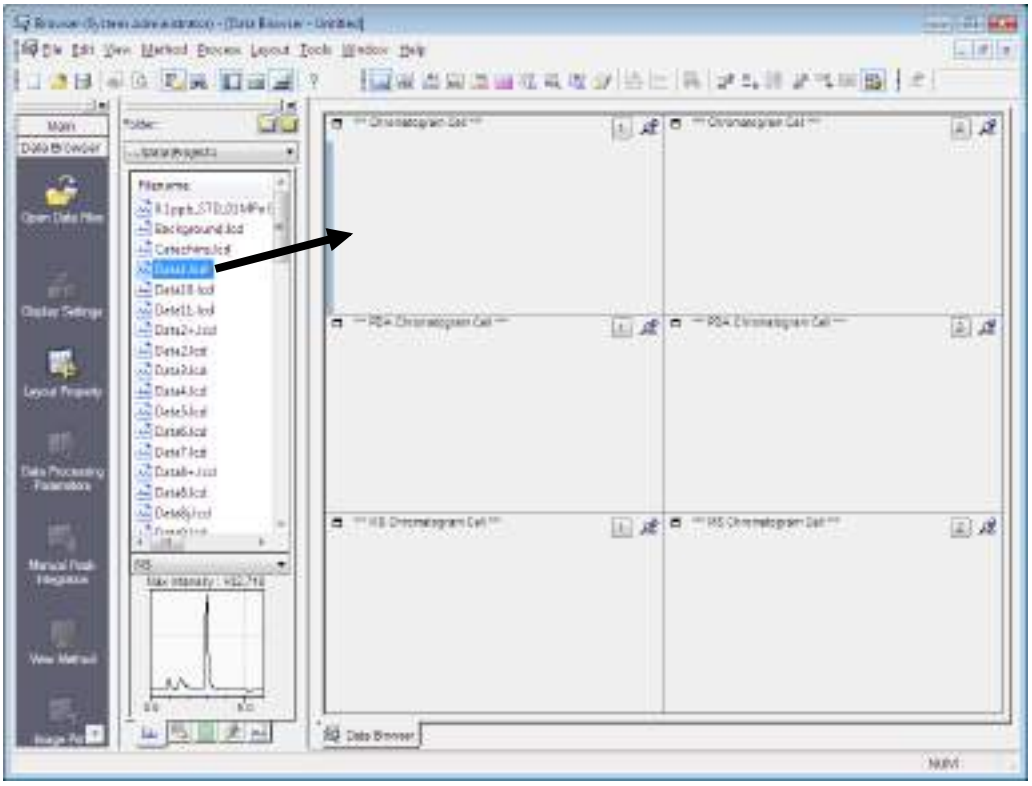


**3** **Click the cell number ( 1 ) that is to be changed, and set the cell number.**

In this example, set the cells in the 1st column to “1” and the cells in the second column to “2”.



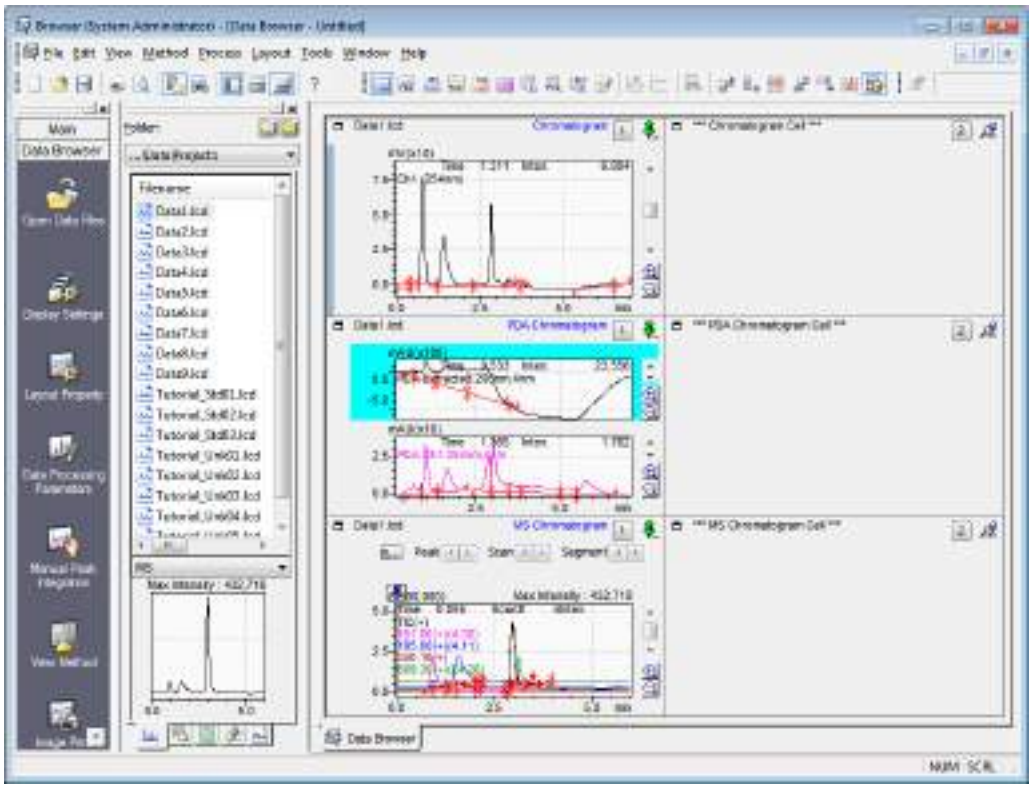
**4** **Drag-and-drop data file 1 onto the number 1 chromatogram cell from the [Data Explorer] sub-window.**



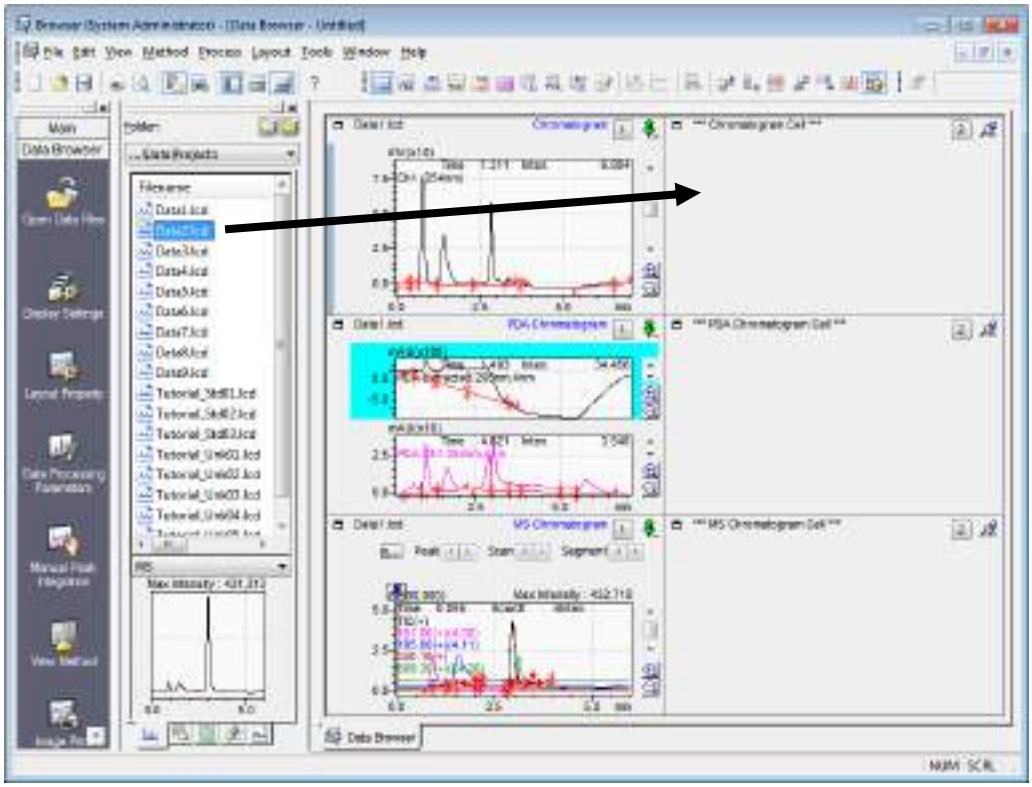
**NOTE**

If a data file is dragged-and-dropped into an [MS Chromatogram] cell that already has a data file in it, a confirmation message is displayed prompting whether it is OK to add data to the cell. Click [Yes] to add the selected data file to the [MS Chromatogram] cell. Click [No] to swap all of the data files in al of the number 1 cells with the new data. In this example, select [No].

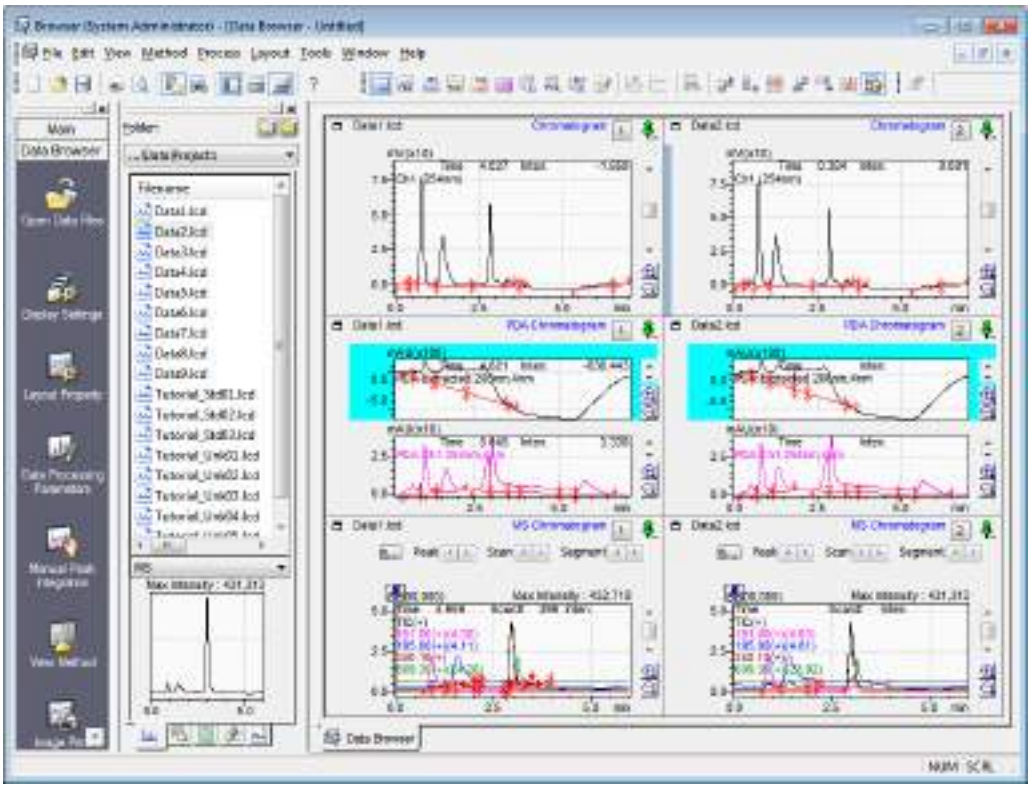
The contents of the data file are displayed in the number 1 cells.



**5** **Drag-and-drop data file 2 onto the number 2 chromatogram cell from the [Data Explorer] sub-window.**



The contents of the data file are displayed in the number 2 cells.



## 12.4.7 Link Content Between Cells

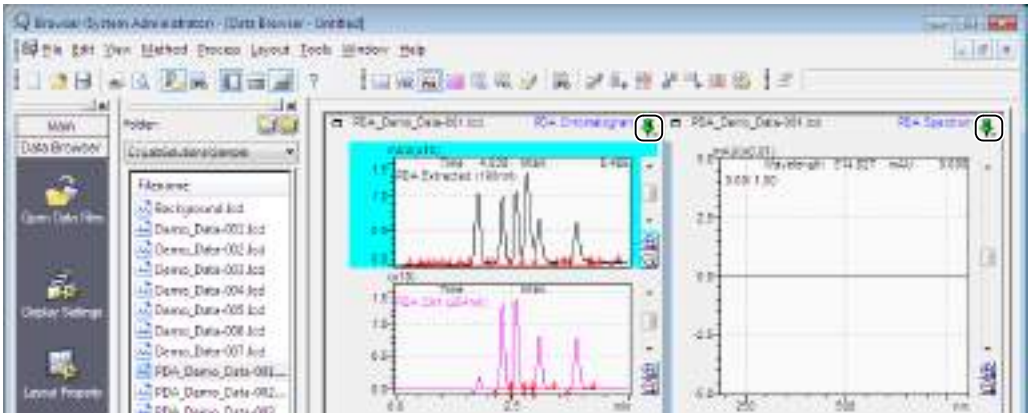
An upright focus pin ( ) indicates that the cell is linked to other cells.

For example, if the [PDA Chromatogram] and [PDA Spectrum] cell are linked and the chromatogram is double-clicked, the displayed spectrum in the [PDA Spectrum] cell is updated.

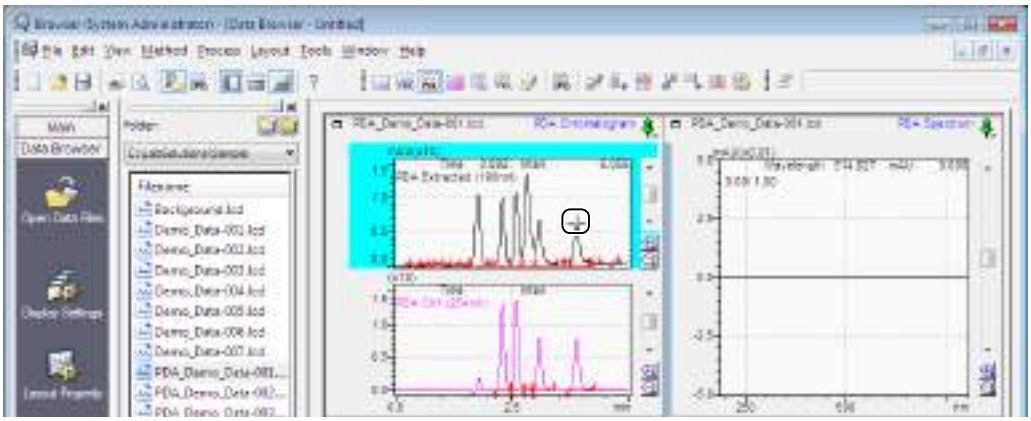
This section describes how to link the [PDA Spectrum] cell display with the [PDA Chromatogram] cell.

**1** **Ensure that the focus pin is upright ( ) on the [PDA Chromatogram] and [PDA Spectrum] cells.**

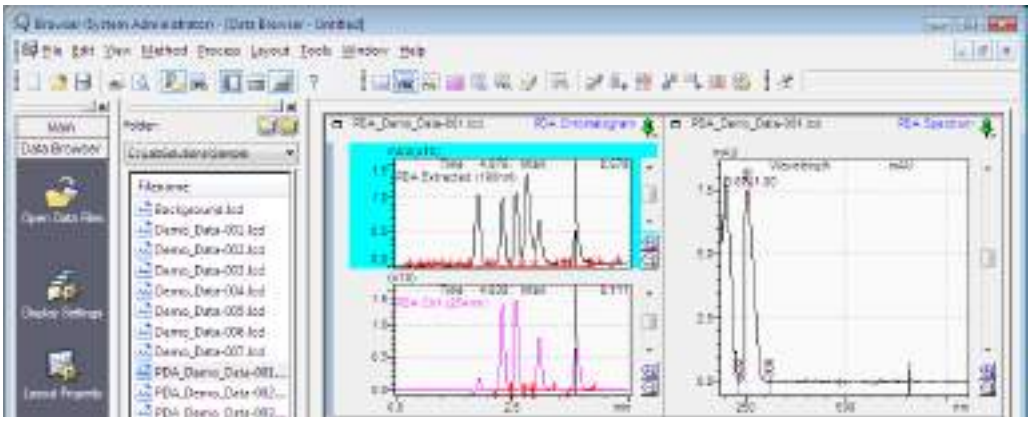
If the focus pin is down ( ), click to change it to the upright state ( ).



## 2 Double-click the desired time position in the [PDA Chromatogram] cell.



The spectrum at that time is displayed in the [PDA Spectrum] cell.



**NOTE**

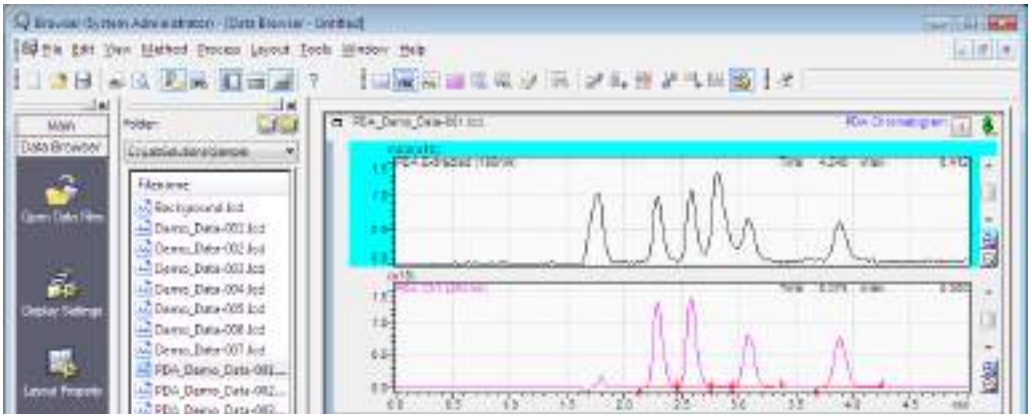
- Depending on the type of cell, the display may be altered to display other information.
- The default state of the focus pin in the cell is upright.
- Click an upright focus pin to disable cell links.

## 12.4.8 Peak Integration on Chromatograms

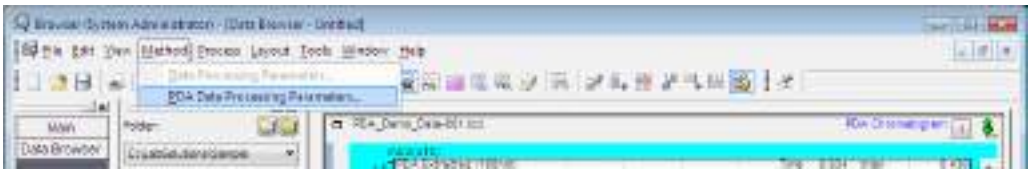
This section describes how to perform peak integration on [PDA Chromatogram] in the [Data Browser] window.

### ■ Perform Peak Integration

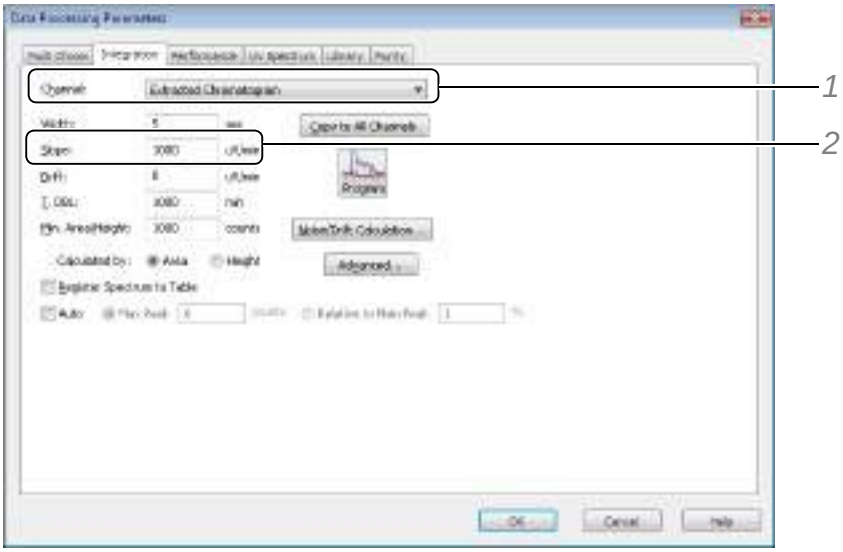
**1** **Open the [PDA Chromatogram] to be integrated.**



**2** **Click [PDA Data Processing Parameters] on the [Method] menu.**



**3** **Click the [Integration] tab, set each of the integration parameters, and click [OK].**




*1* Select the channel to be integrated. In this example, select [Extracted Chromatogram].
*2* Change the [Slope] setting to “1000”.

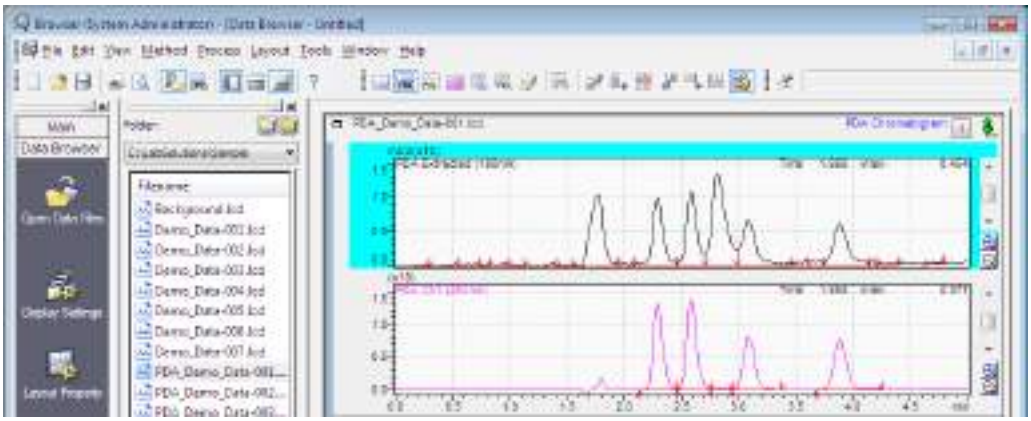
### Reference

Refer to the Data Acquisition & Processing Theory Guide for details on each of the parameters.

**NOTE**

If automatic peak integration is not successful, try manual peak integration. Right-click on the PDA chromatogram and click [Manual Integration Bar] to display the [Manual Integration Bar]. The [Manual Integration Bar] cannot be displayed if an overlaid PDA chromatogram is displayed. Select [Stack] or [Single] to display the [Manual Integration Bar]. Refer to Help for details on the [Manual Integration Bar]

Peak integration is performed on the extracted chromatogram and the results are displayed.
The baseline and peak top comment are displayed on the PDA chromatogram.



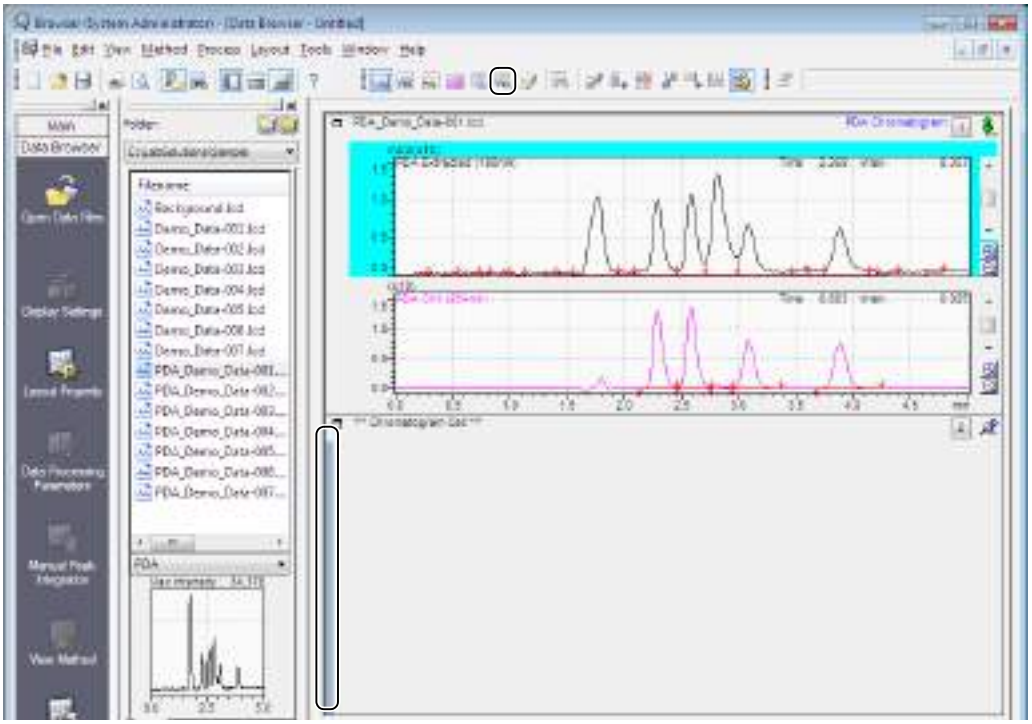
## ■ Examine the Peak Integration Results

The results of peak integration can be examined in the [PDA Peak Table] cell.

This section describes how to change the displayed cell to the [PDA Peak Table] cell to examine the peak integration results of the extracted PDA chromatogram.

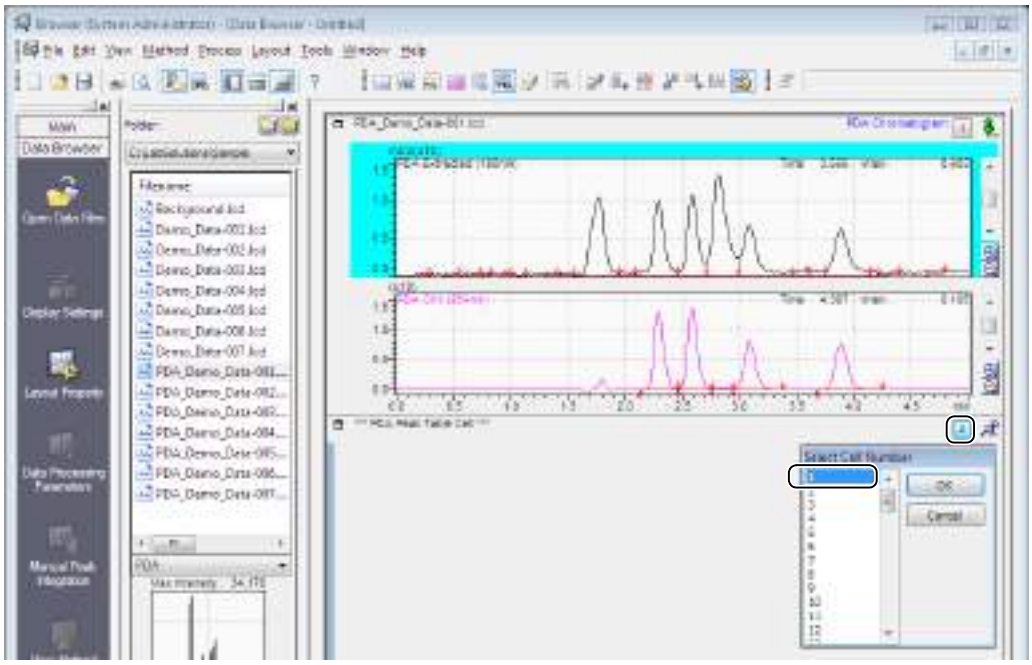
### 1 Select the cell to be changed to the [PDA Peak Table] and click (PDA Peak Table) on the toolbar.

Click the cell to display the focus bar in that cell. Click (PDA Peak Table) on the toolbar to change the cell to the [PDA Peak Table] cell.



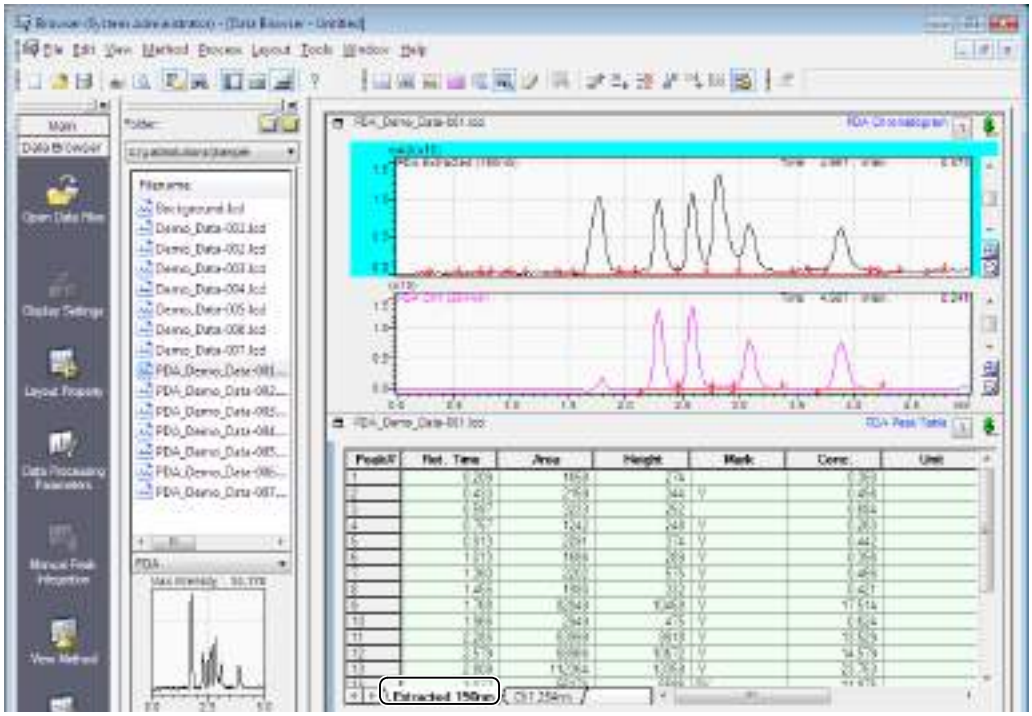
## 2 Click the cell number and select the cell number in the [Select Cell Number] sub-window.

If the cell number is not displayed, refer to *"12.3.1 Use the Cell Fixed Function" P.358* to turn the cell fixed function off.



## 3 Click the [Extracted] tab.

The peak integration results of the extracted PDA chromatogram are displayed.



**NOTE**

The peak integration results of LC chromatograms and MS chromatograms are displayed in the [LC Peak Table] cell and [MS Peak Table] cell, respectively.

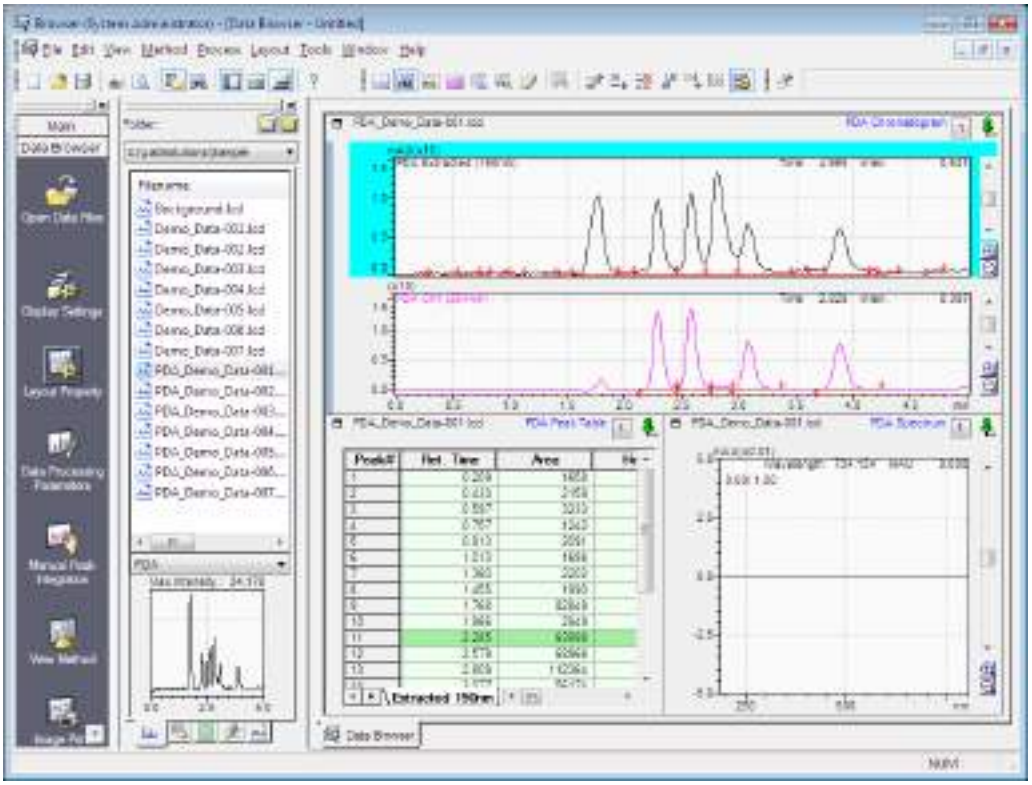
## ■ Link Cells to Check Peak Integration Results

This section describes how to link the [PDA Chromatogram], [PDA Peak Table] and [PDA Spectrum] cells to check peak integration results.

**1** **Position the [PDA Chromatogram], [PDA Peak Table] and [PDA Spectrum] cells as follows.**

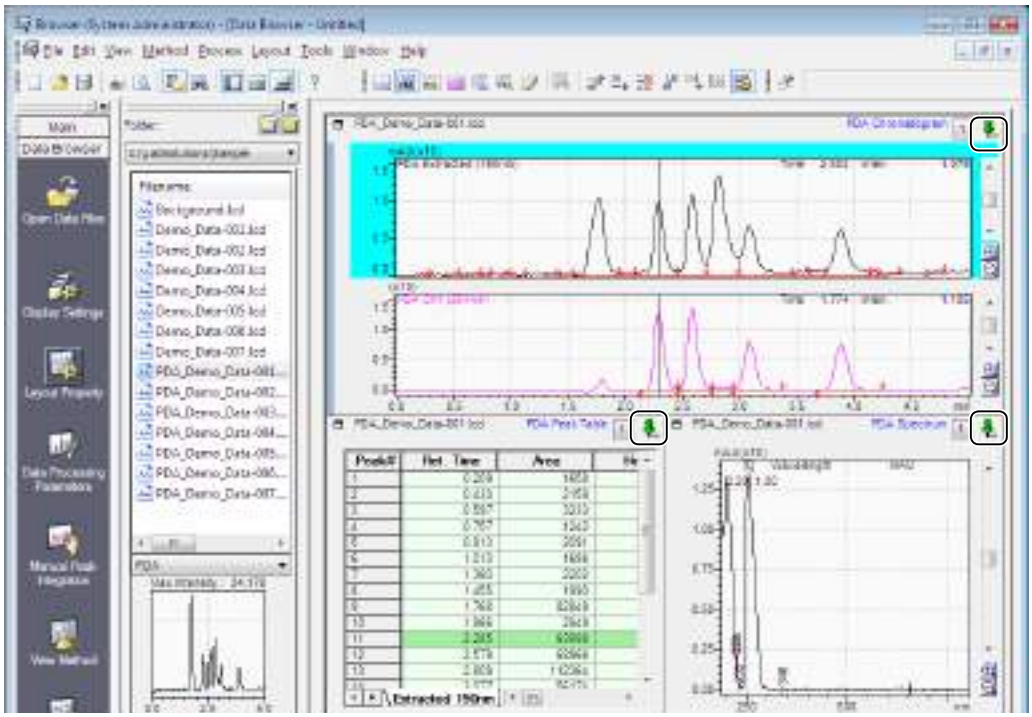
### Reference

Refer to *"12.2 Adjust Layouts" P.354* for details.



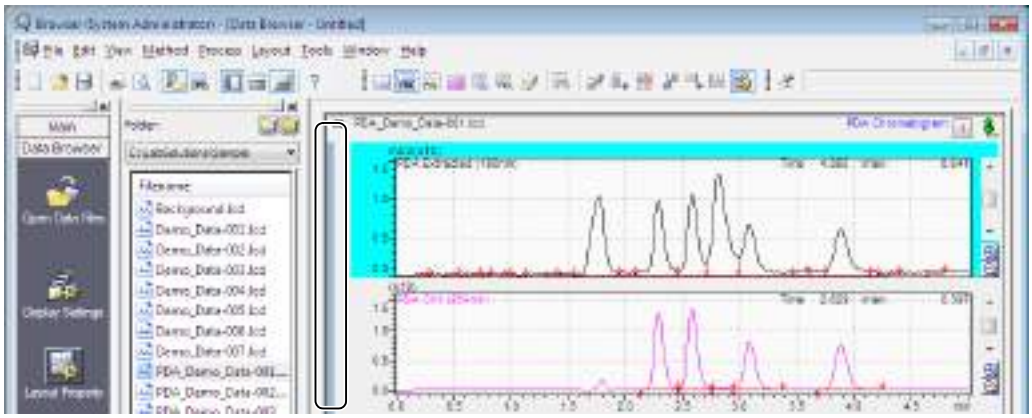
## 2 Ensure that the focus pins of the cells are in the upright ( ) position.

If the focus pin is down ( ), click to change it to the upright state ( ).



## 3 Click the [PDA Chromatogram] cell.

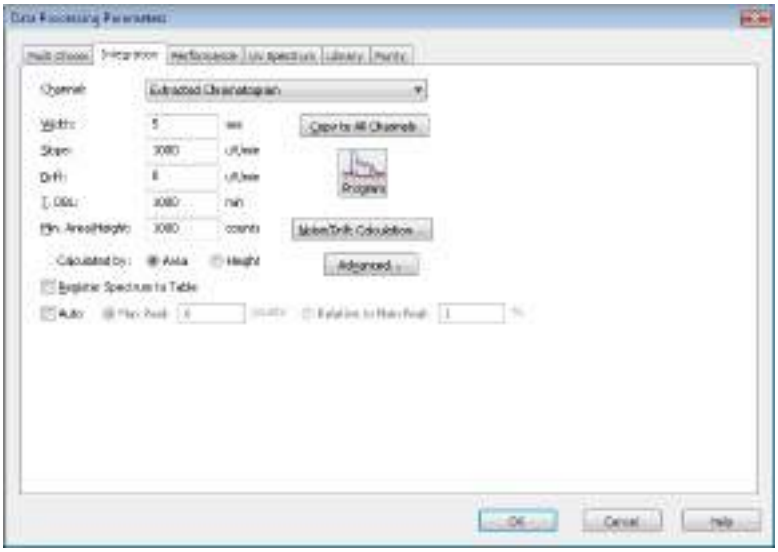
The focus bar is displayed on the [PDA Chromatogram] cell.



## 4 Click [PDA Data Processing Parameters] on the [Method] menu.

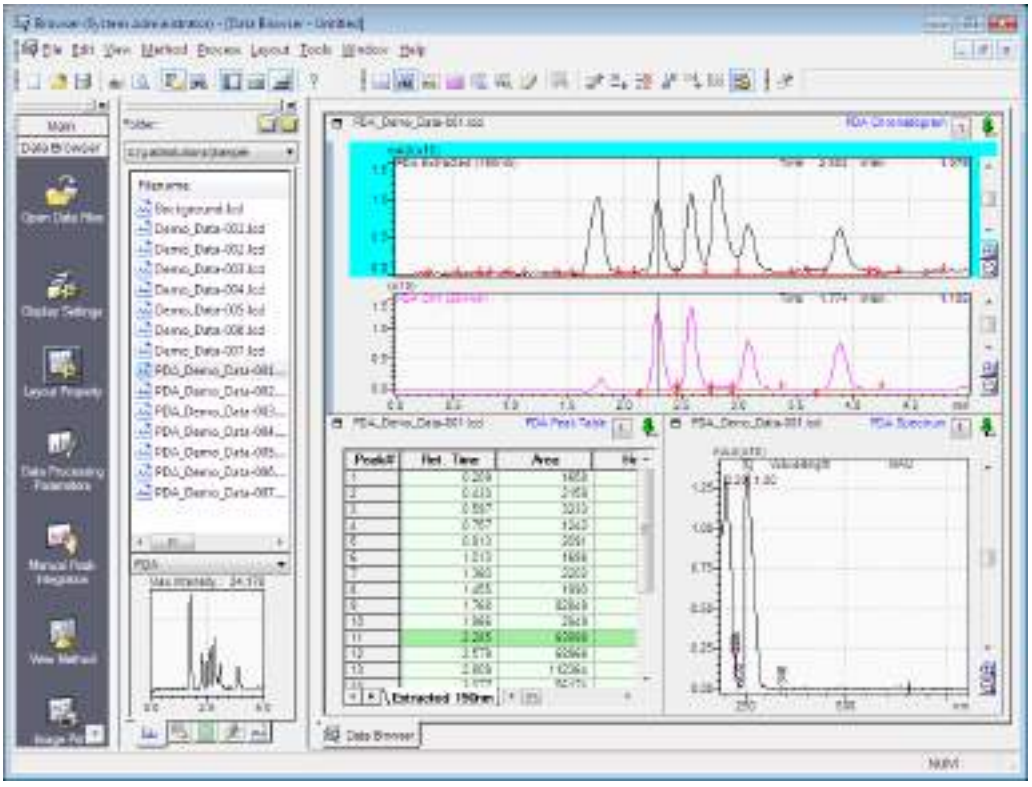
**5** **Enter the parameters in the [Data Processing Parameters] sub-window, and click [OK].**

Peak integration is performed when [OK] is clicked, even if no changes were made in the [Data Processing Parameters] sub-window.



**6** **After peak integration, click a row on [PDA Peak Table].**

The information for that peak is displayed in the [PDA Chromatogram] and [PDA Spectrum] cells.



# 12.5 Print a Browser Report

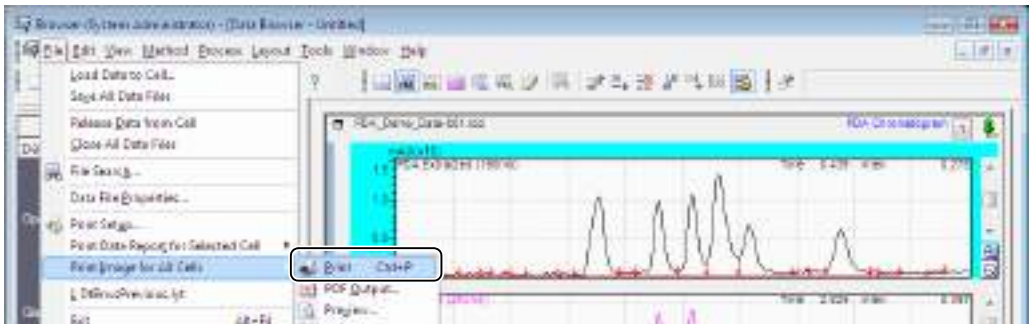
The [Data Browser] window has functions for printing all of the cells or only selected cells. Size, color and other information in the chromatogram and spectrum cells also are reflected in the printout.

## 12.5.1 Print All of the Cells

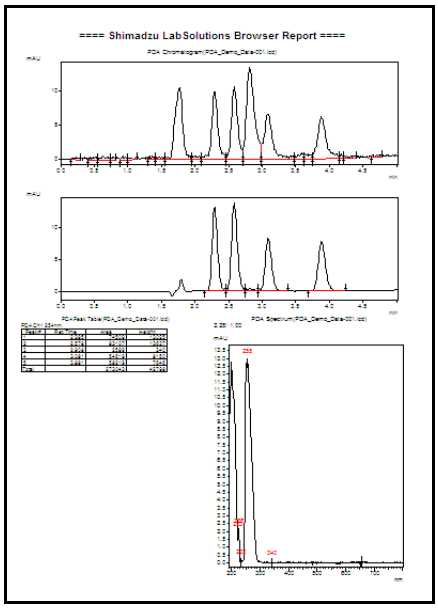
An image of all of the cells currently displayed in the [Data Browser] window can be printed.

This section describes how to print all of the cells.

**1** **Select [Print Image for All Cells] on the [File] menu, and click [Print].**



An image of all of the cells is printed in the preset report layout locations.

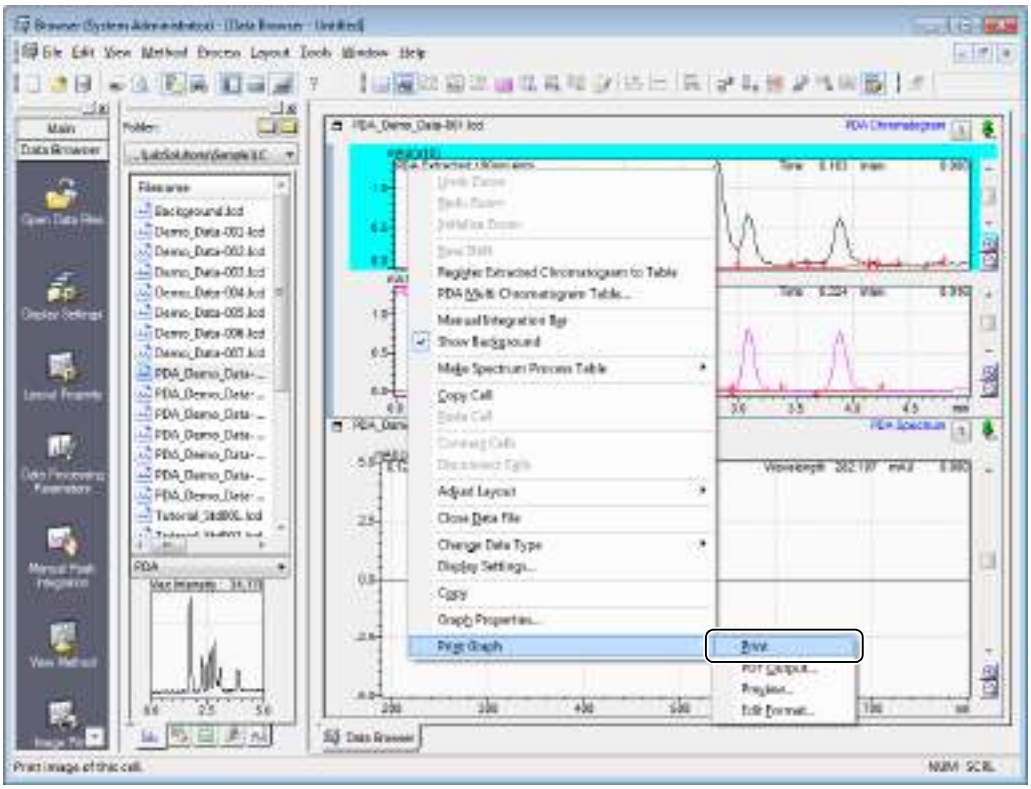


## 12.5.2 Print Selected Cells

An image of the cells currently selected in the [Data Browser] window can be printed.

This section describes how to print the [PDA Chromatogram] cell.

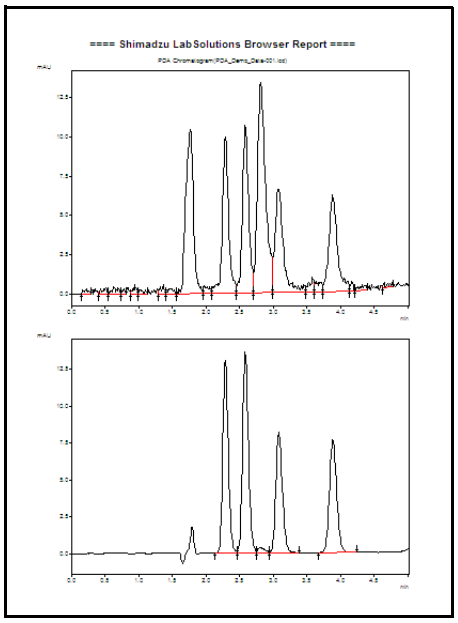
**1** **Right-click on the desired cell, select [Print Graph], and click [Print].**




**NOTE**

The right-click menu changes to [Print Table] or [Print Sample Information] when the cell content is a table or sample information, respectively.

The image of the selected cell is printed.



# 13 Data Comparison

This chapter describes how to overlay multiple data overlaid and perform calculations in the [Data Comparison] window. Up to 16 chromatograms can be overlaid in the [Data Comparison] window for comparison.

Comparison calculations can be performed for the data of any currently specified chromatograms.

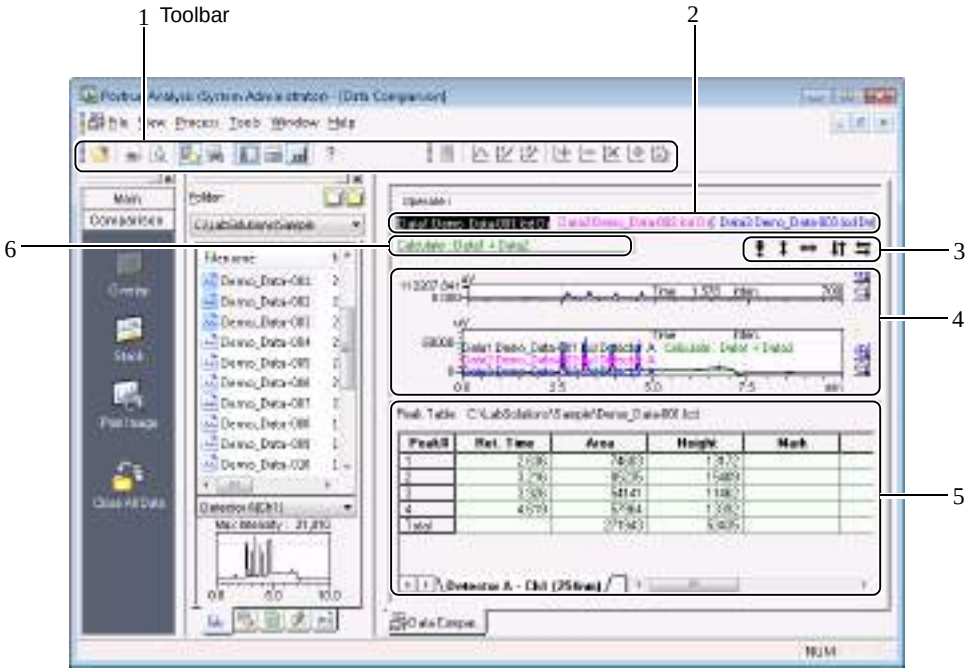
## 13.1 Open the [Data Comparison] Window

This section describes how to overlay the chromatograms of selected data in the [Data Comparison] window.

**1** **Click the (Data Comparison) icon on the assistant bar in the [Postrun Analysis] program.**

# 13.2 [Data Comparison] Window Description

This section describes how to view and use the [Data Comparison] window.




| No. | Explanation |
|---|---|
| 1 | Displays the [Standard] and [Data Comparison] toolbars. |
| 2 | Displays the information for the displayed data file.<br>Right-click on the data file information and click [Close] to close the data file. |
| 3 | Use these buttons to expand, reduce or moves a selected chromatogram to the top, bottom, left or right.<br>• To move a chromatogram up/down or left/right, click (Move Up/Down) or (Move Left/Right) and drag the chromatogram to the move destination position.<br>• Click (Base Point) to expand or reduce a chromatogram and the click the position of the base point on the chromatogram to determine that point. Next, click (Zoom Up/Down) or (Zoom Left/Right), and drag the chromatogram to the expand/reduce destination point. The chromatogram is expanded or reduced to that point. |
| 4 | Displays the chromatogram of the open data file as [Full Chromatogram] or [Zoomed Chromatogram]. Three view methods are available, [Overlay], [Stack] and [Base Shift]. |
| 5 | Displays the Peak Table of the selected chromatogram. |
| 6 | Displays calculation formulas for operations performed between the data of selected chromatograms. |

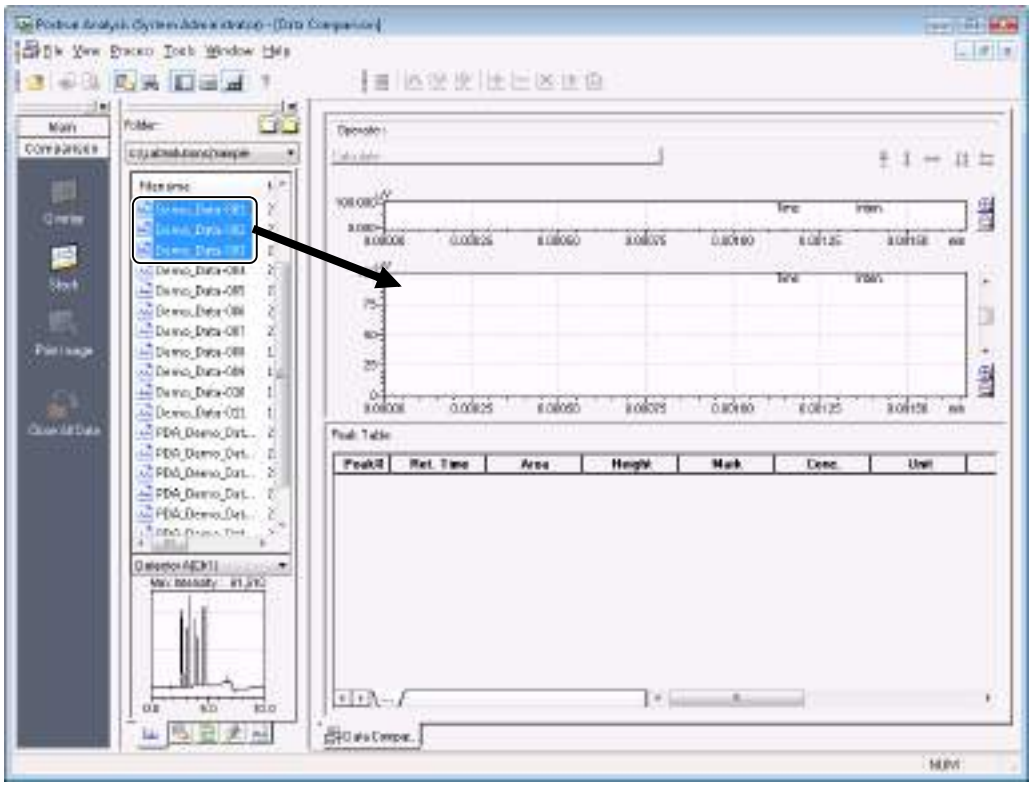
**NOTE**

- Right-click on the chromatogram and select [Base Shift] to shift the displayed chromatograms by an equal interval.
- Right-click on the chromatogram and select [Copy] to paste the chromatograms into other applications as image files.
- Select [Close] on the [File] menu, then select [All Data] to close all of the open data.

# 13.3 Overlay Multiple Data

This section describes how to display the chromatograms of selected data overlaid in the [Data Comparison] window.

**1** **Select the data file to overlay in the [Data Explorer] sub-window, and drag-and-drop that file onto the [Data Comparison] window.**



The chromatogram and Peak Table of the data files are displayed in the [Data Comparison] window.

**NOTE**

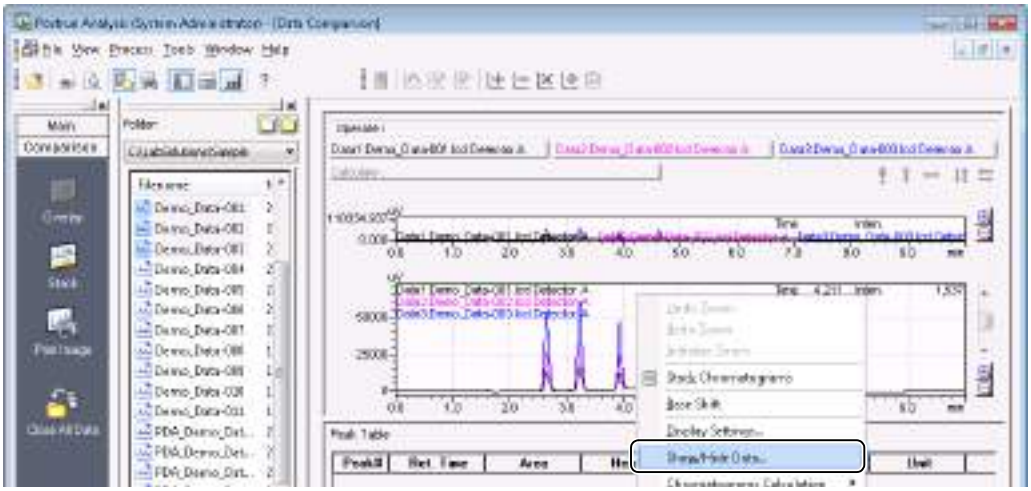
- A sub-window opens for channel selection when displaying a data file obtained by data acquisition on multiple channels. Select the checkbox of the channel to display.
- Data files obtained by a PDA detector cannot be displayed overlaid in the [Data Comparison] window.
  To display in the [Data Comparison] window, select [Export Data] on the [File] menu in the [PDA Data Analysis] window, click [Export Chromatogram to Data File] and extract the multi chromatogram.
- Click the (Stack) icon on the [Comparison] assistant bar to display chromatograms in a stacked format.

# 13.4 Perform Calculations on Chromatograms

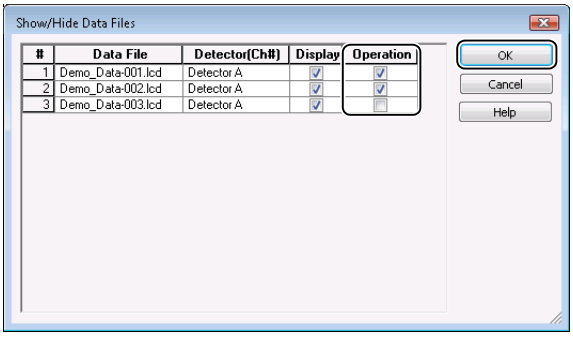
Specify any displayed chromatograms to perform arithmetic calculations (addition/subtraction/multiplication/division) on the data.

This section describes how to perform arithmetic operations on 2 chromatograms.

**1** **Right-click on [Chromatogram View], and click [Show/Hide Data].**



**2** **Select [Operation] to perform the arithmetic operation on the data, and click [OK].**



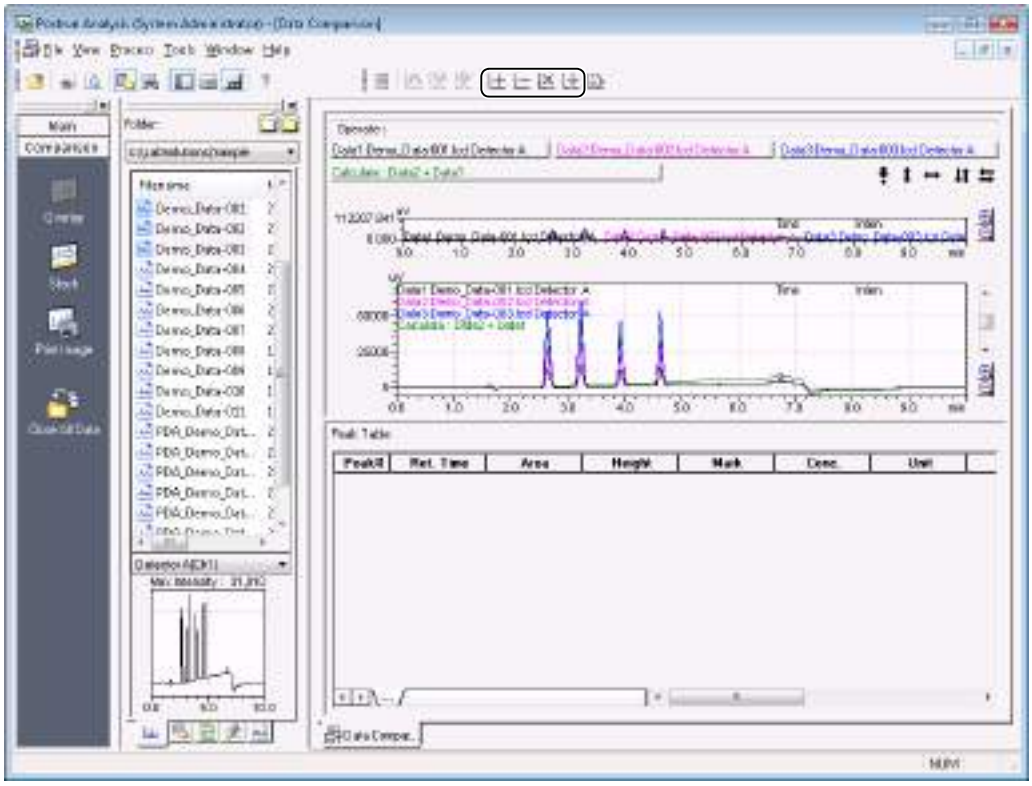

**NOTE**

Arithmetic operation can only be executed between 2 chromatograms.
An error occurs if 3 or more chromatograms are selected.

**3** **Click the desired arithmetic operation ( ) on the toolbar.**

The arithmetic operation is performed on the data of the selected chromatograms, and an additional green chromatogram is displayed.

The calculation formula can be checked by Calculate : Data2 + Data1.



**NOTE**

- Click (Reverse Data Order) on the toolbar to change Calculate : Data2 + Data1 to Calculate : Data1 + Data2 so that the calculation data is reversed.
- Right-click on [Chromatogram View], and select [Save Processed Data] to save the calculation result.

# 14 LC Calibration Curves

This chapter describes how to make calibration curves and check calibration curve information.

There are two ways to make a calibration curve:

- Automatic creation by batch processing
- Manual creation in the [Calibration Curve] window

This section describes how to make calibration curves automatically by postrun batch processing at *"14.1 Calibration Curves by Postrun Batch"* and manually in the [Calibration Curve] window at *"14.2 [Calibration Curve] Window"*.

**Reference**

- MS data cannot be processed in the [Calibration Curve] window. Check and edit calibration curves for MS data in the [Quant Browser] window. See*"11 Quant Browser" P.327*.
- See *"3.6 Create a Calibration Curve to Quantitate an Unknown Sample" P.71* for details on automatically making calibration curves using realtime batch.

## 14.1 Calibration Curves by Postrun Batch

Use postrun batch to automatically make a calibration curve using the data file of a standard sample that has already been acquired.

This section describes how to set data processing parameters and Batch Table items to make calibration curves.

### 14.1.1 Edit the Data Processing Parameters

This section describes how to edit the data processing parameters of method files using standard samples data.

**1** **Click the (Data Analysis) icon on the [Main] assistant bar in the [Postrun Analysis] program.**

**2** **Drag-and-drop the standard sample data file that has already been acquired onto the [Data Analysis] window from the [Data Explorer] sub-window.**

**3** **Click the (Wizard) icon on the [Data Analysis] assistant bar.**

**4** **Refer to *"4.5.1 Compound Table Wizard" P.116* to set the data processing parameters using the Compound Table Wizard.**

**5** **Click View (View Mode) in [Method View].**

The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the analysis results in [Chromatogram View] and [Results View].

**6** **Click the (Apply to Method) icon on the [Data Analysis] assistant bar.**

The parameters are exported to the method file.

**Reference**

For details, see *"4.7 Save (Export) to Method Files" P.126*.

## 14.1.2 Edit Batch Tables

### ■ Create Batch Tables

This section describes how to create batch tables. There are two ways to create a Batch Table according to how data is acquired.

- New Batch Table
- Load the Batch Table used for data acquisition

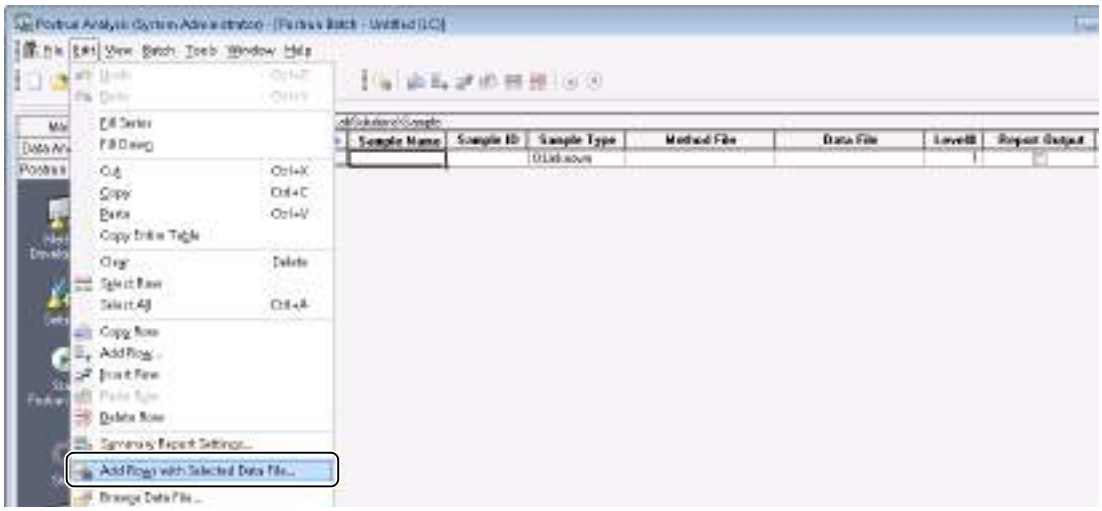
### New Batch Table

**1** **Click the (Postrun Batch) icon on the [Main] assistant bar in the [Postrun Analysis] program.**

**NOTE**

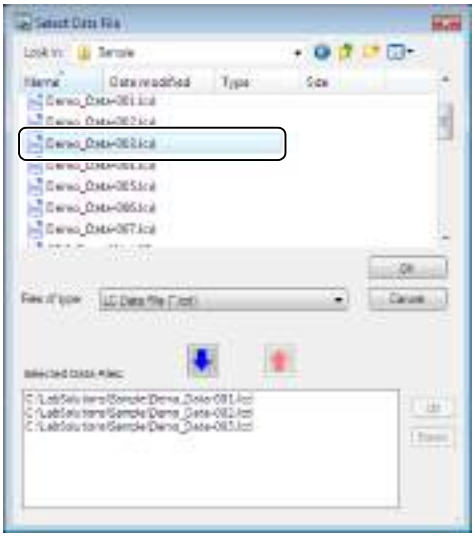
If the (Postrun Batch) icon is not displayed on the assistant bar, click Main on the assistant bar title.

**2** **Click [Add Rows with Selected Data File] on the [Edit] menu.**



**3** **Select the data file name and then click .**

The data file name is displayed in the [Selected Data Files] box. Repeat this procedure to select all of the files required for postrun batch.



The Batch Table is created from the information in the selected data file.

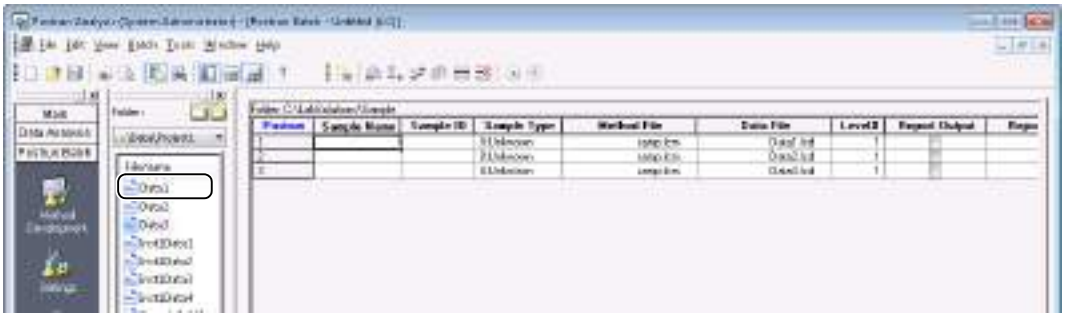
## Load a Batch Table Used for Data Acquisition

**1** **Click the (Postrun Batch) icon on the [Main] assistant bar in the [Postrun Analysis] program.**

**NOTE**

If the (Postrun Batch) icon is not displayed on the assistant bar, click Main on the assistant bar title.

**2** **Drag-and-drop the batch file used for data acquisition onto the [Postrun Batch] window from the [Data Explorer] sub-window.**



## ■ Set the Sample Type

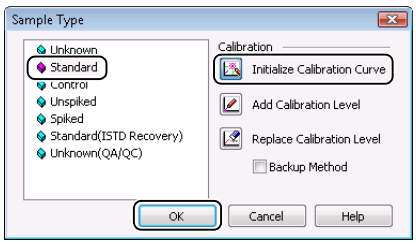
Set the type of sample to measure.

In the case of a standard sample, set the first standard sample to [Initialize Calibration Curve] and the next standard sample to [Add Calibration Level]. The default setting [0: Unknown] is used for unknown samples.

**1** **Click the [Sample Type] cell of the initial standard sample.**

| Postrun | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# | Report Output | Repo |
|---|---|---|---|---|---|---|---|---|
| 1 | STD1 | | 0:Unknown | samp.lcm | Data1.lcd | 1 | | |
| 2 | STD2 | | 0:Unknown | samp.lcm | Data2.lcd | 1 | | |
| 3 | STD3 | | 0:Unknown | samp.lcm | Data3.lcd | 1 | | |

**2** **Click [Standard], select [Initialize Calibration Curve] and click [OK].**

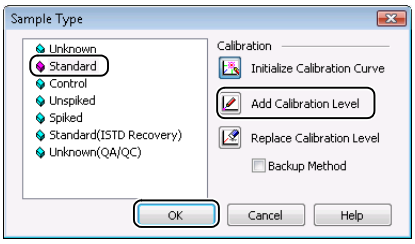



The initial cell for the sample type is displayed as [1: Standard (i)].

**3** **Click the [Sample Type] cell of the next standard sample.**

| Postrun | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# | Report Output | Repo |
|---|---|---|---|---|---|---|---|---|
| 1 | STD1 | | 1:Standard (i) | samp.lcm | Data1.lcd | 1 | | |
| 2 | STD2 | | 0:Unknown | samp.lcm | Data2.lcd | 1 | | |
| 3 | STD3 | | 0:Unknown | samp.lcm | Data3.lcd | 1 | | |

**4** **Click [Standard], select [Add Calibration Level] and click [OK].**




The cell for the sample type is displayed as [1: Standard].
Repeat steps 3 and 4 for multiple standard samples.

| Postrun | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# | Report Output | Repo |
|---|---|---|---|---|---|---|---|---|
| 1 | STD1 | | 1:Standard:(I) | samp.lcm | Data1.lcd | 1 | | |
| 2 | STD2 | | 1:Standard | samp.lcm | Data2.lcd | 1 | | |
| 3 | STD3 | | 0:Unknown | samp.lcm | Data3.lcd | 1 | | |

## ■ Setting the Level #

Set the standard sample [Level#] according to the concentration value in the Compound Table of the method file. The calibration points are created from the level number of the Compound Table and the area and height values of the preset standard sample.

**NOTE**
[Level#] values are not used for unknown samples, even if they are set.

**1** **Click the [Level#] cell for the standard sample.**

| Postrun | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# | Report Output | Repo |
|---|---|---|---|---|---|---|---|---|
| 1 | STD1 | | 1:Standard:(I) | samp.lcm | Data1.lcd | 1 | | |
| 2 | STD2 | | 1:Standard | samp.lcm | Data2.lcd | 1 | | |
| 3 | STD3 | | 0:Unknown | samp.lcm | Data3.lcd | 1 | | |

**2** **Enter the level number.**

| Postrun | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# | Report Output | Repo |
|---|---|---|---|---|---|---|---|---|
| 1 | STD1 | | 1:Standard:(I) | samp.lcm | Data1.lcd | 1 | | |
| 2 | STD2 | | 1:Standard | samp.lcm | Data2.lcd | 4 | | |
| 3 | STD3 | | 0:Unknown | samp.lcm | Data3.lcd | 1 | | |

The level number. is changed.

**3** **Set the [Level#] cell for other standard samples.**

## 14.1.3 Postrun Analysis Using Batch Tables

**1** **Click the (Start Postrun Batch) icon on the [Postrun Batch] assistant bar.**

Postrun batch is started.

| Postrun | Sample Name | Sample ID | Sample Type | Method File | Data File | Level# | Report Output | Repo |
|---|---|---|---|---|---|---|---|---|
| 1 | STD1 | | 1:Standard:(I) | samp.lcm | Data1.lcd | 1 | | |
| 2 | STD2 | | 1:Standard | samp.lcm | Data2.lcd | 2 | | |
| 3 | STD3 | | 0:Unknown | samp.lcm | Data3.lcd | 1 | | |

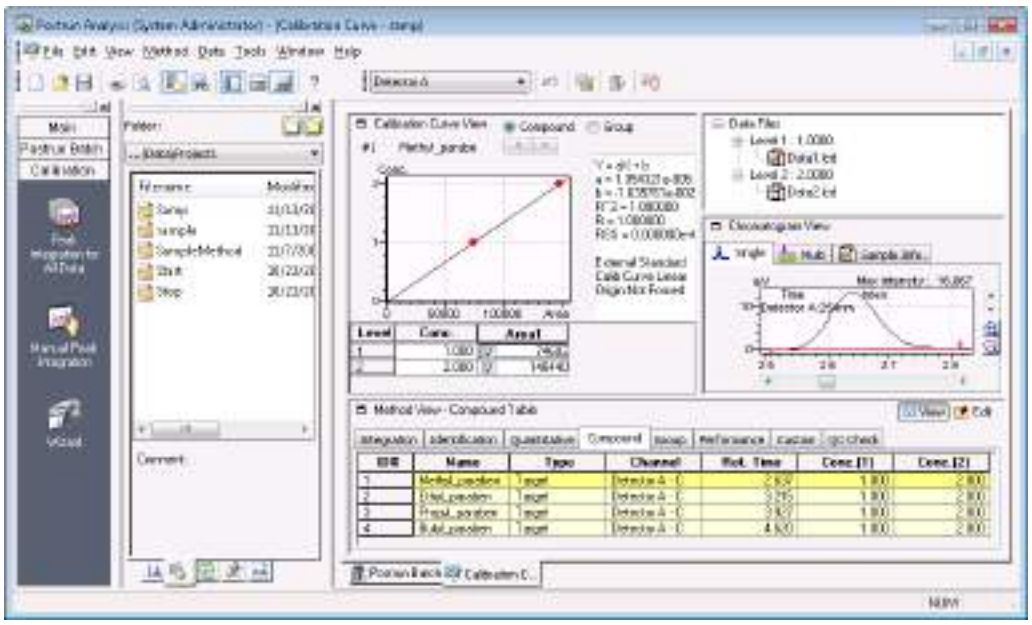
## 14.1.4 Check Calibration Curves

Check whether the calibration curve has been successfully drawn in the [Calibration Curve] window in *"14.1.3 Postrun Analysis Using Batch Tables"*.

**1** **Select the [Method File] cell in the batch table, and click the (Method Development) icon on the [Postrun Batch] assistant bar.**

| Postrun | Sample Type | Method File | Data File | Level# | Report Output | Report Forma |
|---|---|---|---|---|---|---|
| 1 | 1:Standard:(I) | samp.lcm | Data1.lcd | 1 | | |
| 2 | 1:Standard | samp.lcm | Data2.lcd | 2 | | |
| 3 | 0:Unknown | samp.lcm | Data3.lcd | 1 | | |

**2** **Check the calibration curve in the [Calibration Curve] window.**



# 14.2 [Calibration Curve] Window

Check calibration curves made in realtime or postrun batch in the [Calibration Curve View] window and make calibration curves by manually adding calibration points.

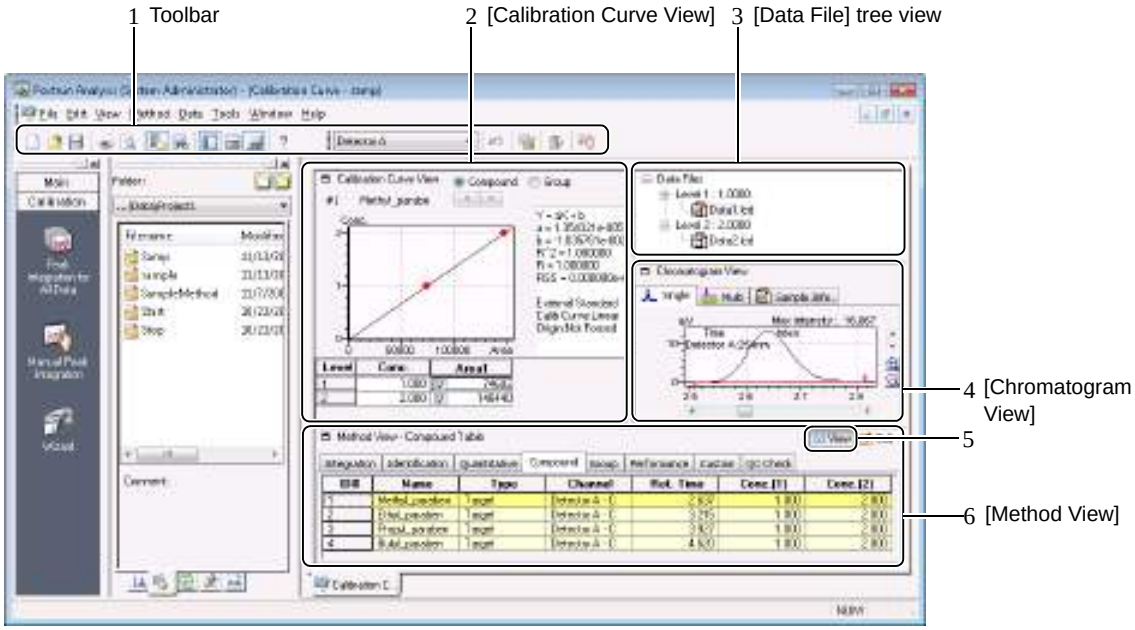
The [Calibration Curve] window has four views, [Calibration Curve View] displays calibration curves, [Method View] displays the data processing parameters, the [Data Files] tree view displays the data files used for calibration curves, and [Chromatogram View].

## 14.2.1 [Calibration Curve] window Description

This section describes how to view the [Calibration Curve] window.

**NOTE**

The layout of each view can be changed in the [Calibration Curve] window.
Two modes are provided for the display layout, [Normal Mode] and [Many Ingredients Mode], which is used when there are many identified peaks.




| No. | Explanation |
|---|---|
| 1 | Displays the [Standard] and [Calibration Curve] toolbars. |
| 2 | Displays a calibration curve graph, calibration curve information and Calibration Table. |
| 3 | Displays the data files for the individual levels used to make the calibration curve.<br>Calibration points for each level can be added or deleted.<br>Add data files by dragging-and-dropping them from the [Data Explorer] sub-window. |
| 4 | Displays the chromatograms and sample information of the data files used to make the calibration curve. |
| 5 | Parameters are displayed in the [View] mode, and can be changed in the [Edit] mode. |
| 6 | Displays the data processing parameters in the method file. |

## 14.2.2 Make Calibration Curves in the [Calibration Curve] Window

This section describes how to manually make calibration curves.

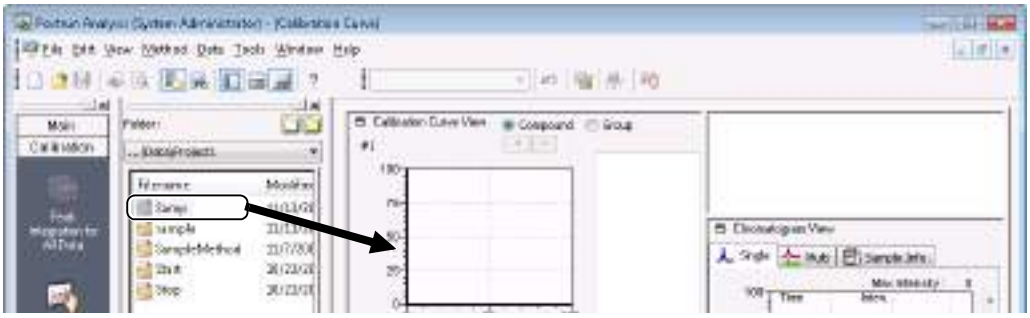
Data processing parameters must be set before calibration curves can be manually created in the [Calibration Curve] window.

**1** **Click the (Calibration Curve) icon on the [Main] assistant bar in the [Postrun Analysis] program.**

**2** **Select the method file.**

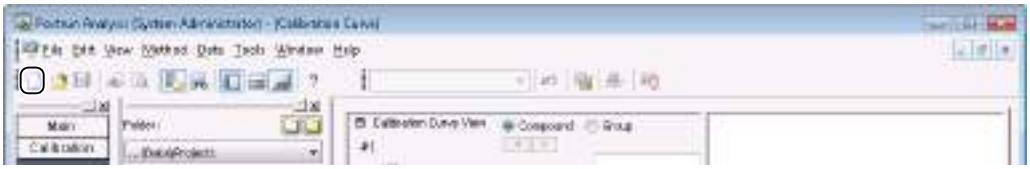
- Existing method file

1 Drag-and-drop the method file onto the [Calibration Curve] window from the [Data Explorer] sub-window.



- New method file

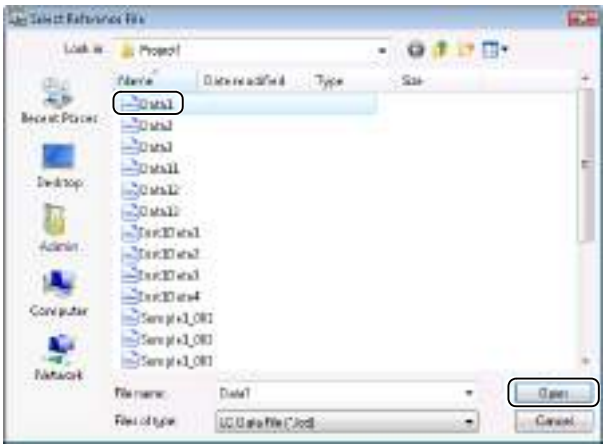
1 Click the (New) button on the toolbar.



The following message is displayed.

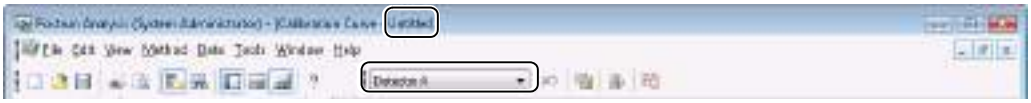
2 Click [OK].

3 Select the method file used for data acquisition or a method file with the same system configuration, and click [Open].

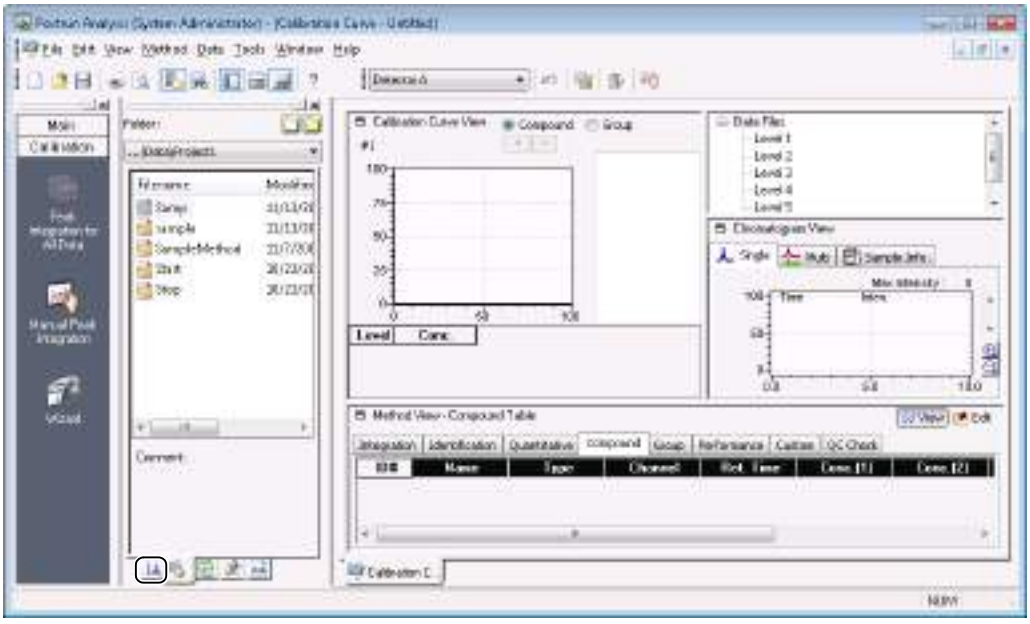


The detector is set based on the system configuration information in this file.

The [Calibration Curve] window changes to [Untitled].



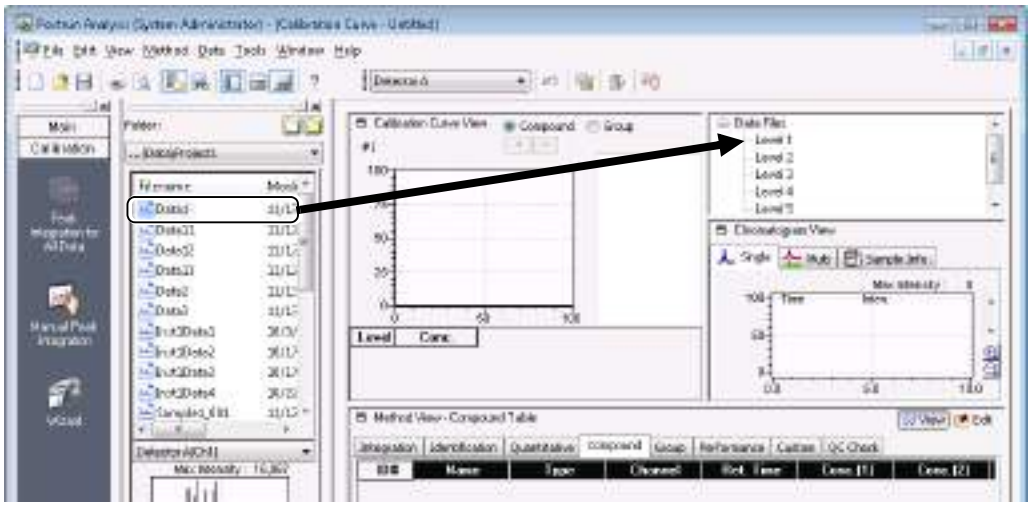
**3 Click the [Data] tab at the bottom of the [Data Explorer] sub-window.**



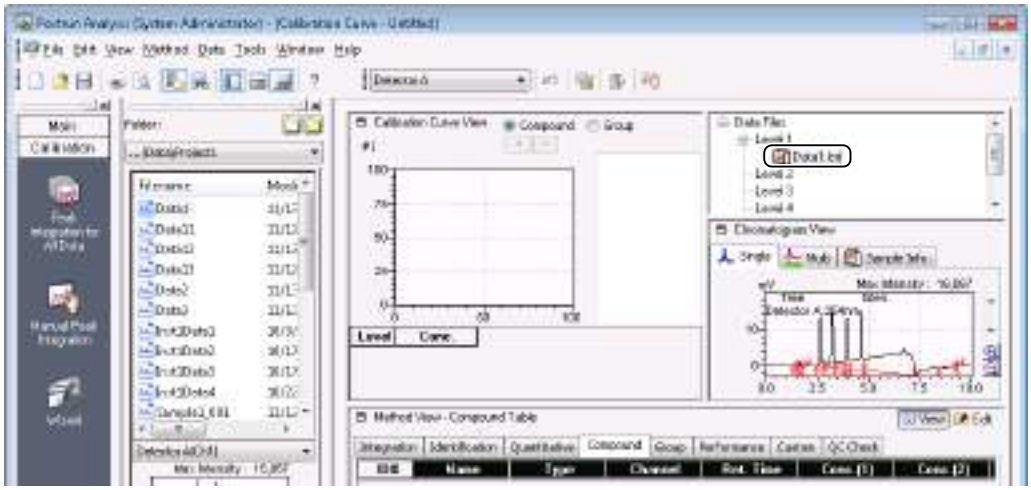
**4** **Drag-and-drop the data file of the standard sample onto the target level in the [Data Files] tree view from the [Data Explorer] sub-window.**

**NOTE**

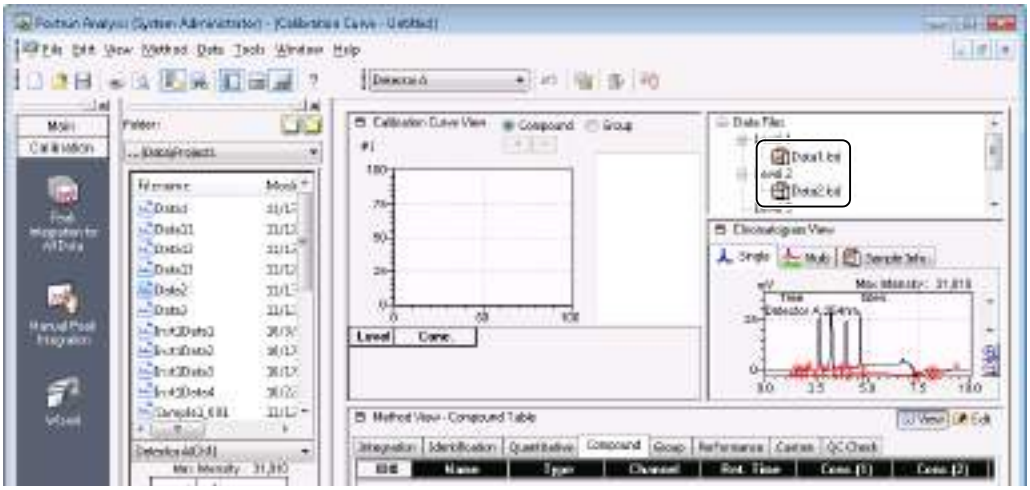
Drag-and-drop the data file onto the same level position as the concentration set in the Compound Table of the method file.



The data file is added to the level.

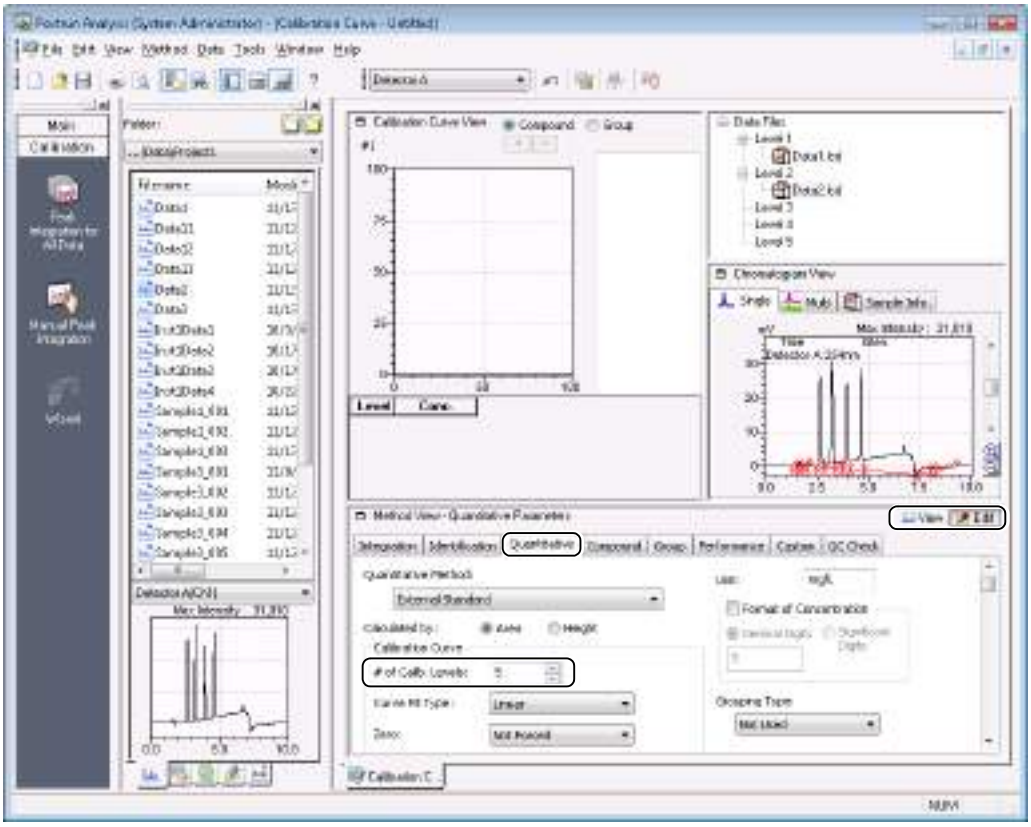


Repeat the above step and drag-and-drop the additional standard sample data file onto the target level when multiple standard samples are used.



**NOTE**

Set the [# of Calib. Levels] on the [Quantitative] tab in the [Method View] to increase the number of levels in the calibration curve.



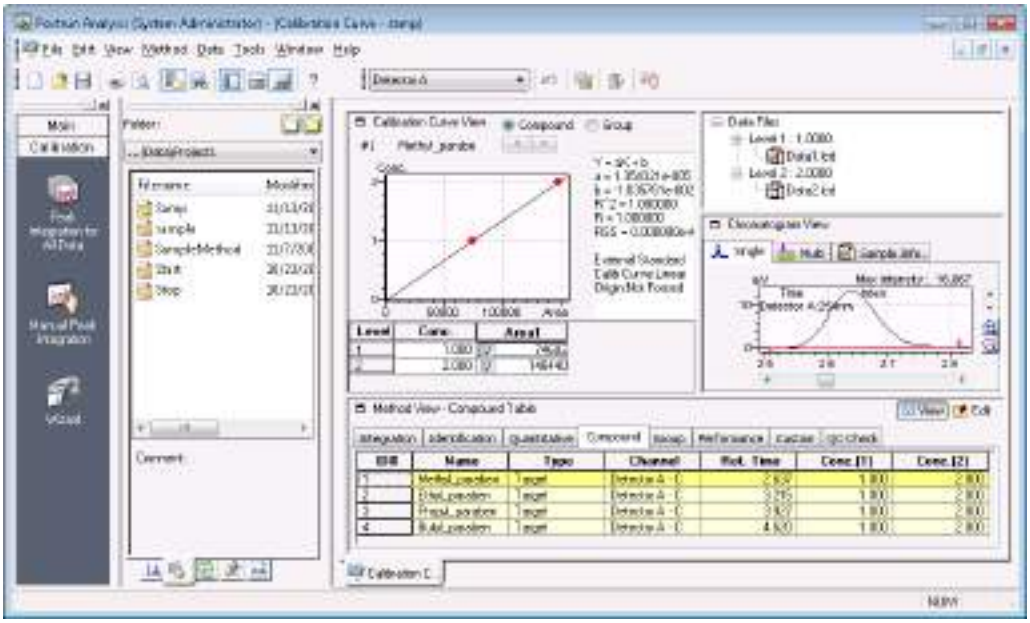
**5** **Click the**  **(Wizard) icon on the [Calibration] assistant bar.**

**6** **Refer to *"4.5.1 Compound Table Wizard" P.116* to set the data processing parameters using the Compound Table Wizard.**

**7** **Click** 

**(View Mode) in [Method View].**

Data processing is performed on the data loaded in the [Data Files] tree view according to the parameters set in the Compound Table Wizard.



**8** **Click the**  **(Save) button on the toolbar.**

The method file and the data file(s) in the [Data Files] tree view are saved.

# 15 Appendix

This chapter describes how to locate operation details on the Help menu or in the online manuals. Use this information in the event that you are having problems with software operation, and the basic operations in software screens.

## 15.1 Operation Problems

This software provides the Help menu and online manuals. Use the Help menu and online manuals to learn more about software operations or the terms displayed on screen.

This section describes how to use the Help menu and online manuals.

### 15.1.1 Help

Use the following procedures to open the Help menu.

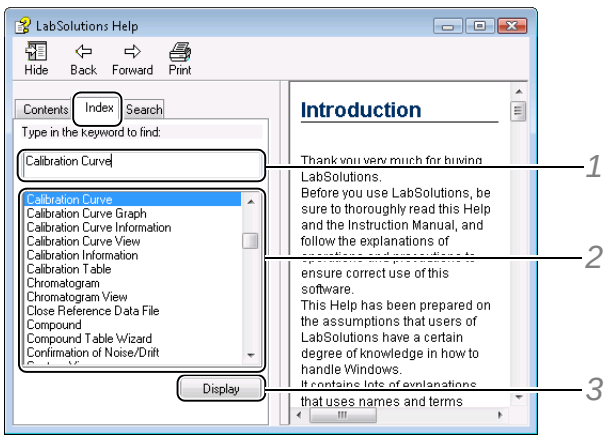
| Type of Operation | Operation Procedures |
|---|---|
| [Help] | Click [Help] on the sub-window.<br>The section Help for the current sub-window is displayed. |
| (Help) | Click (Help) on the toolbar. |
| [Help] menu | Click [Contents] on the [Help] menu. |
| [F1] key | Press the [F1] key on your keyboard. To locate the details relating to the current sub-window. |

#### ■ Keyword Search

If the term or parameter is unknown, enter a keyword to perform a search, and a list of topics that match the keyword is displayed. This allows for review of Help topics that pertain to the terms and parameters.

**1** **Open Help.**

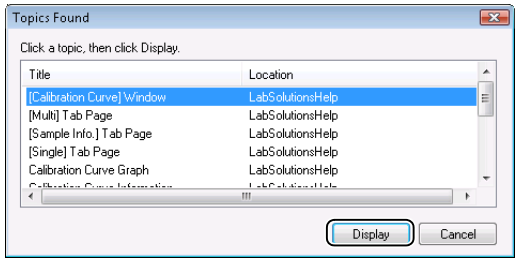
**2** **Click the [Index] tab, and execute the search.**



1 Enter the keyword to search for, and press the [Enter] key on your keyboard.
Topics matching the keyword are displayed in an alphabetical order.
2 Click the topic.
3 Click [Display].
The contents of the selected topic is displayed.

**NOTE**

- The [Topic Found] sub-window opens if there are multiple matching keywords. Select the desired keyword in the list in this sub-window, and click [Display].



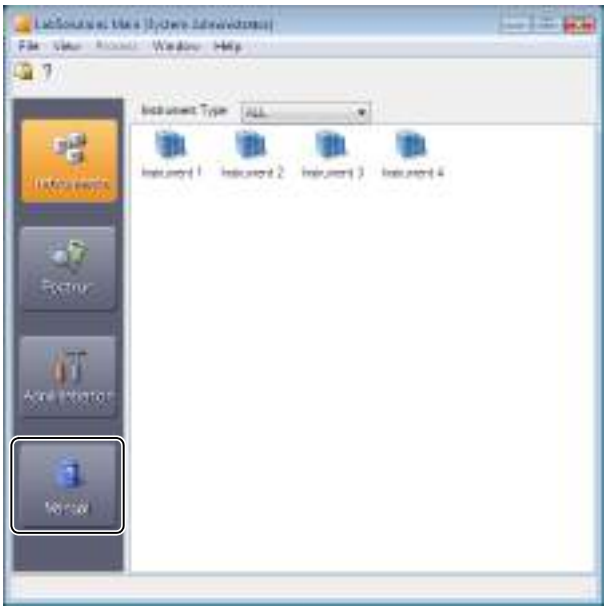

- Use the [Search] tab in the Help window to search the entire text of the Help topic for the keyword terms.

## 15.1.2 Online Manuals

The "Operators Guide", "System Users Guide", "Data Acquisition & Processing Theory Guide", "Getting Started Guide" and other online manuals are installed in PDF format when this software is installed.

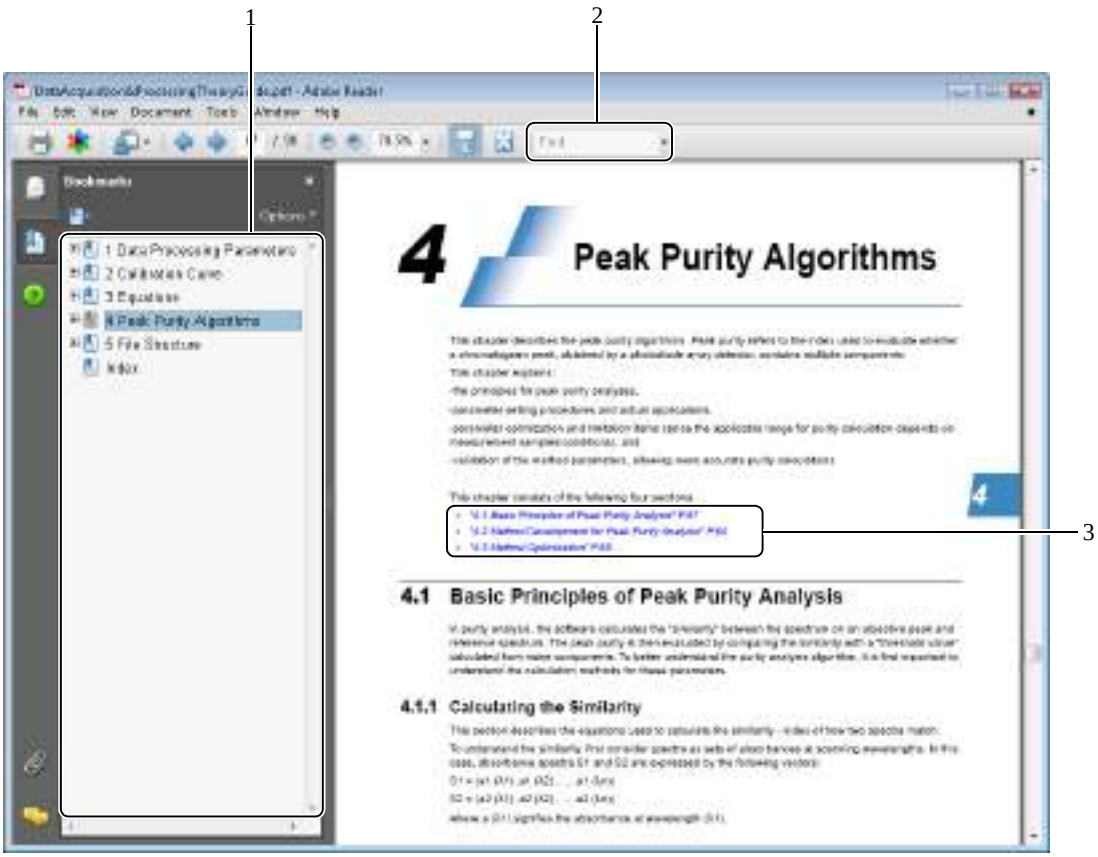
This section describes how to display online manuals.

**1 Click the  icon in the [LabSolutions Main] window.**



## 2 Click the icon of the desired instruction manual.

This opens Adobe Acrobat® Reader® and the instruction manual.




| No. | Explanation |
|---|---|
| 1 | Go directly to the desired page by clicking the hierarchically structured bookmarks (table of contents). |
| 2 | Search for desired terms. |
| 3 | Go directly to a related page by clicking the references or the terms in blue. |

**NOTE**

- The “Operators Guide” online manual can also be opened by clicking [Online Manual] on the [Help] menu in the window.
- Adobe Reader® is required to open online manuals.
- Visit Adobe's website for details on Adobe Reader®.

# 15.2 Common Screen Operations

The windows, assistant bars, toolbars and other graphical user interface elements in this software can be customized.

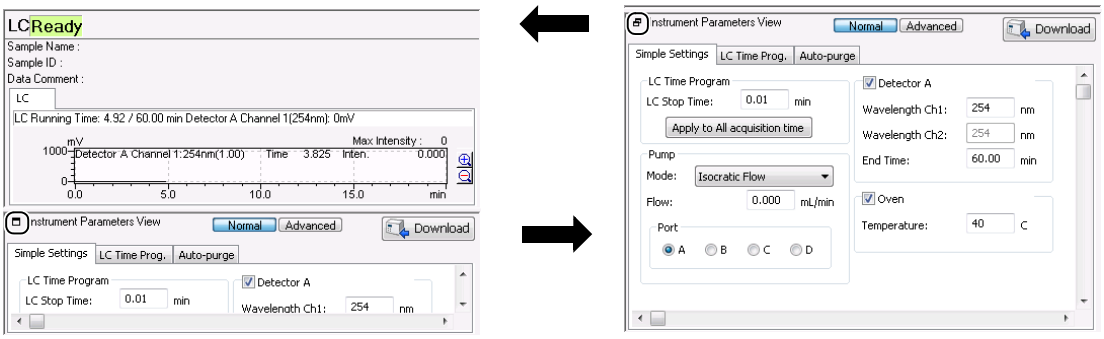
## 15.2.1 Resize the View

Many of the windows such as [Data Acquisition] and [Data Analysis] are comprised of sections (views) that are separated by dividers. Drag the dividers to resize the views to make on-screen operations more efficient.

### ■ Resize Icons

To resize a view, click (Full Size) in each view. This changes the normal size display to its full size. Alternatively, click (Normal Size) to return the full size display to its normal size.

**Normal size** **Full size**

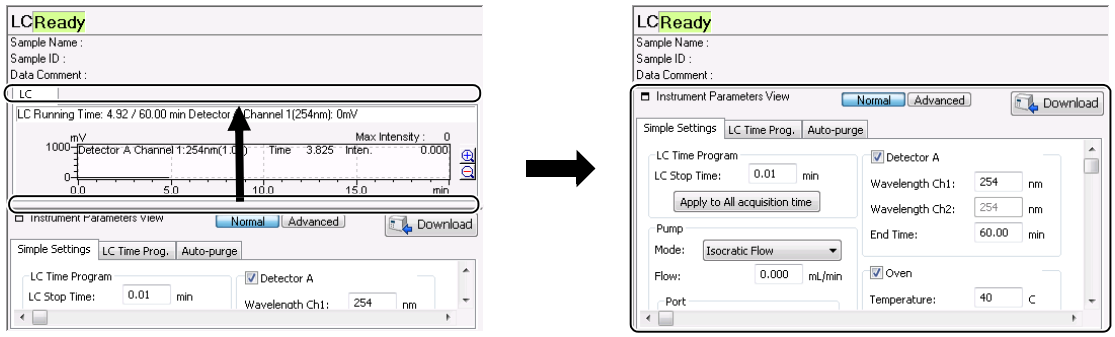



**NOTE**

[Results View] and [Method View] in the [Data Analysis] window contain a (Wide Size) icon for displaying views at the full horizontal size and a (Normal Size) icon to return the wide size view to the normal size.

### ■ Drag the Dividers to Resize Views

Views can be resized as desired by dragging the dividers of each view.



## 15.2.2 Customize Windows

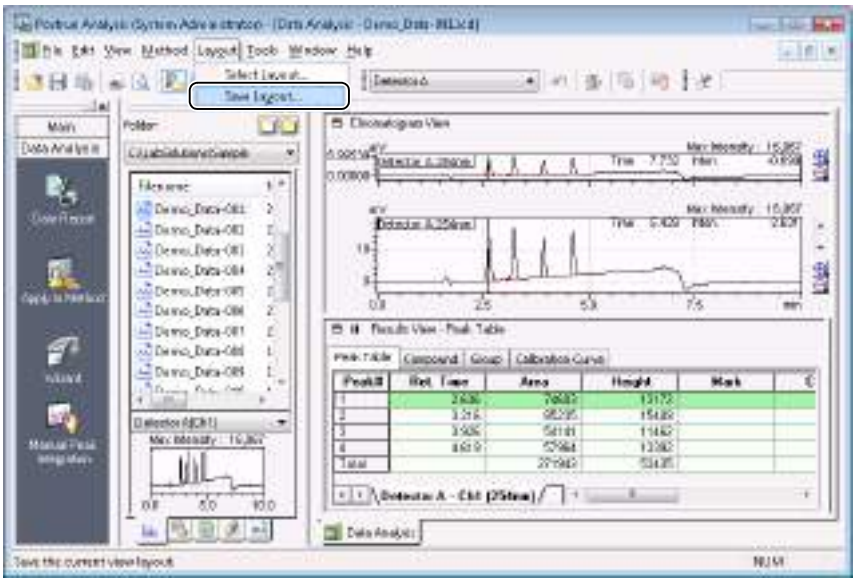
This software allows a customized view layout for a specific operation to be saved.

For example, since the [Data Analysis] and [PDA Data Analysis] windows have many views, data can be more easily analyzed by saving various layouts with unwanted views hidden.

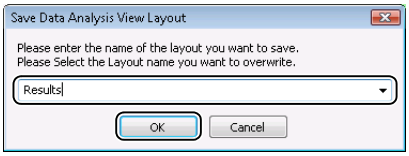
This section describes the procedure for saving the [Data Analysis] window layouts.

### ■ Save Layouts

**1** **Click [Save Layout] on the [Layout] menu.**



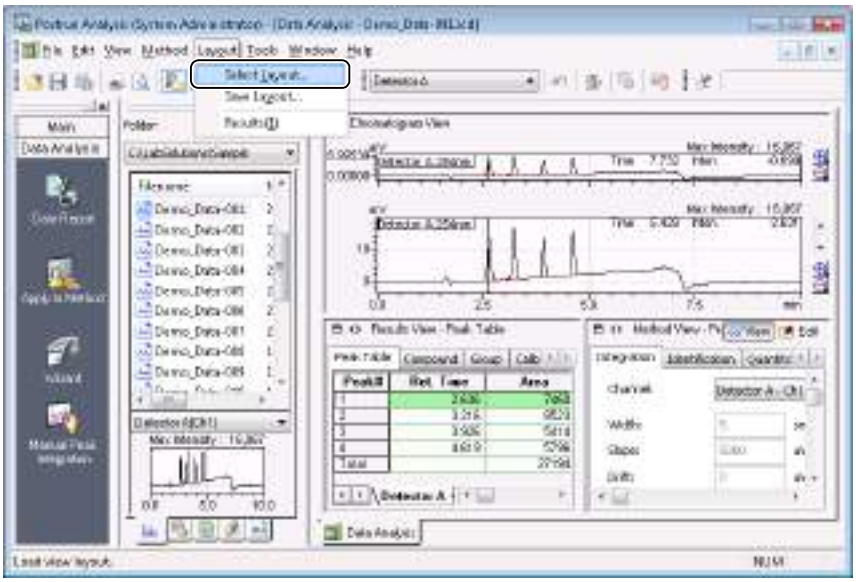

**2** **Enter the name of the layout, and click [OK].**



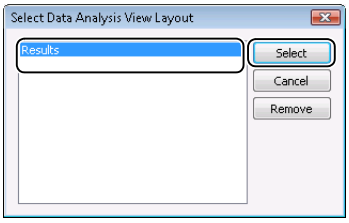

The layout of the currently open window is saved.

## ■ Open a Saved Layout

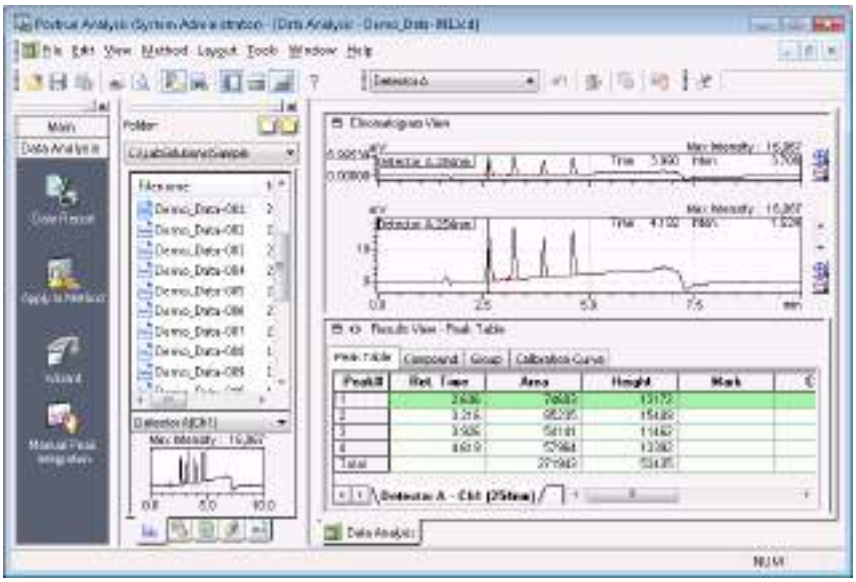
**1** **Click [Select Layout] on the [Layout] menu.**



**2** **Select the name of the layout, and click [Select].**




The window is opened using the selected layout.



## 15.2.3 Customize Assistant Bars

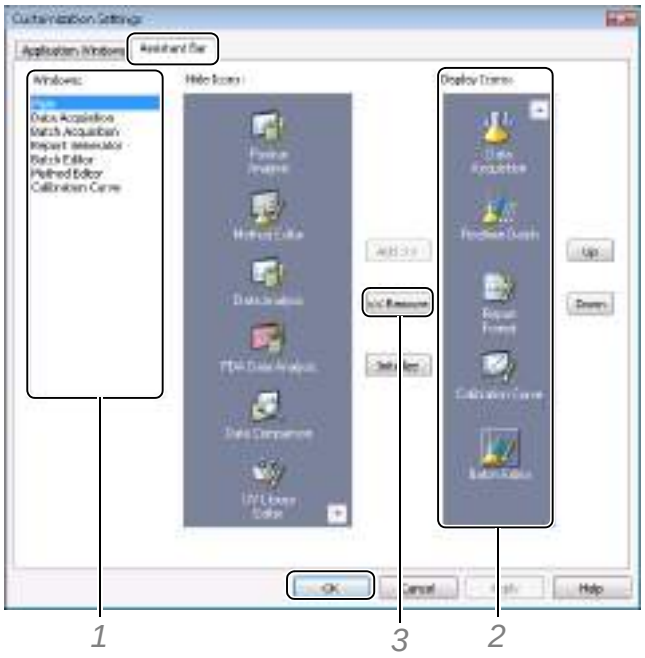
This software allows the addition or deletion of icons displayed on assistant bars to customize assistant bars for specific operations.

This section describes how to delete the [Batch Editor] icon from the [Main] assistant bar in the [Realtime Analysis] program.

**1** **Open the [Data Acquisition] window.**

**2** **Select [Customization] on the [Tools] menu, and click [Customization Settings].**


**3** **Click the [Assistant Bar] tab, select the icon to delete, and then click [OK].**




1 Select [Main] at [Windows].
2 Select the [Batch Editor] icon at [Display Icons].
3 Click [Remove] to move the [Batch Editor] icon to [Hide Icons].

The [Batch Editor] icon is no longer displayed on the [Main] assistant bar in [Realtime Analysis].

**NOTE**

- It is only possible to customize the icons for the functions used in each window of the [Realtime Analysis], [Postrun Analysis] and [Browser] programs. Customize windows by editing [Available] on the [Application Windows] tab.
- Select the icon at [Display Icons], and click [Up] or [Down] to change the display order of icons on the assistant bar.

## 15.2.4 Customize Toolbars

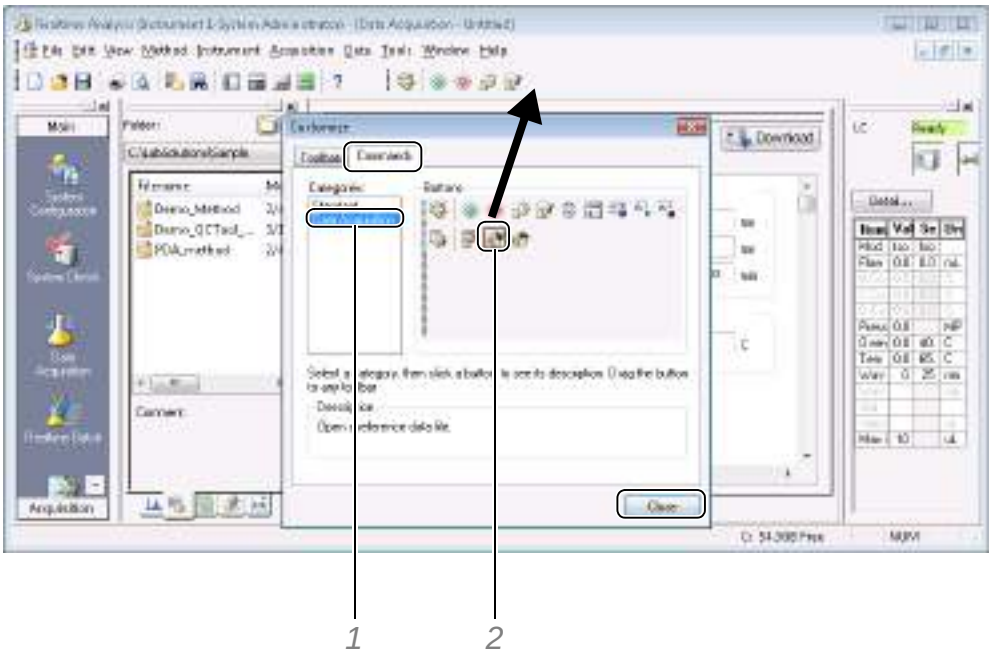
This software allows the addition or deletion of icons displayed on toolbars to customize the toolbars for specific operations.

This section describes how to add the [Open Reference Data File] icon to the [Data Acquisition] toolbar.

**1** **Open the [Data Acquisition] window.**

**2** **Select [Customization] on the [Tools] menu, and click [Toolbar Customization Settings].**

**3** **Click the [Command] tab, customize the [Data Acquisition] toolbar, and then click [Close].**




*1* Select [Data Acquisition] at [Categories].

*2* Drag-and-drop  (Open Reference Data File) onto the [Data Acquisition] toolbar.

The button is added to the [Data Acquisition] toolbar.

**NOTE**

- Deselect the check mark of a displayed toolbar on the [Toolbar] tab to hide a toolbar.
- Drag-and-drop a button on the toolbar to an area outside of the toolbar to delete the button from the toolbar.

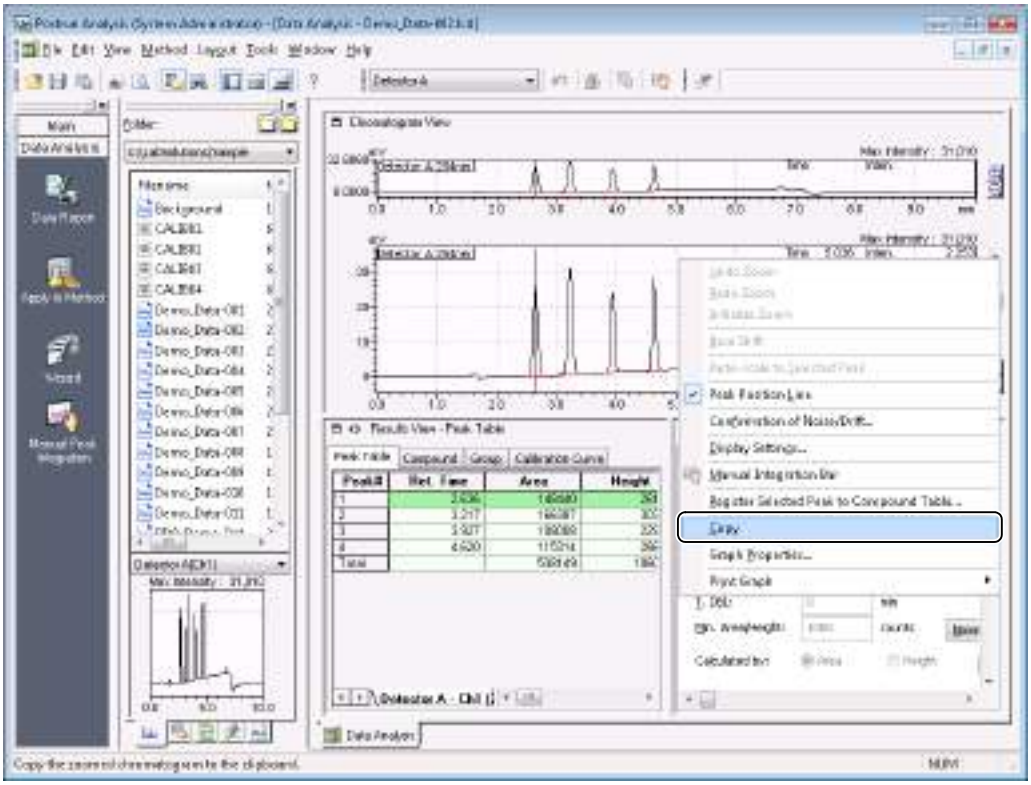
## 15.2.5 Copy Sub-Windows to the Clipboard

Chromatograms and Calculation Results Tables displayed in the sub-windows of this software can be copied to the Clipboard and pasted to other application software.

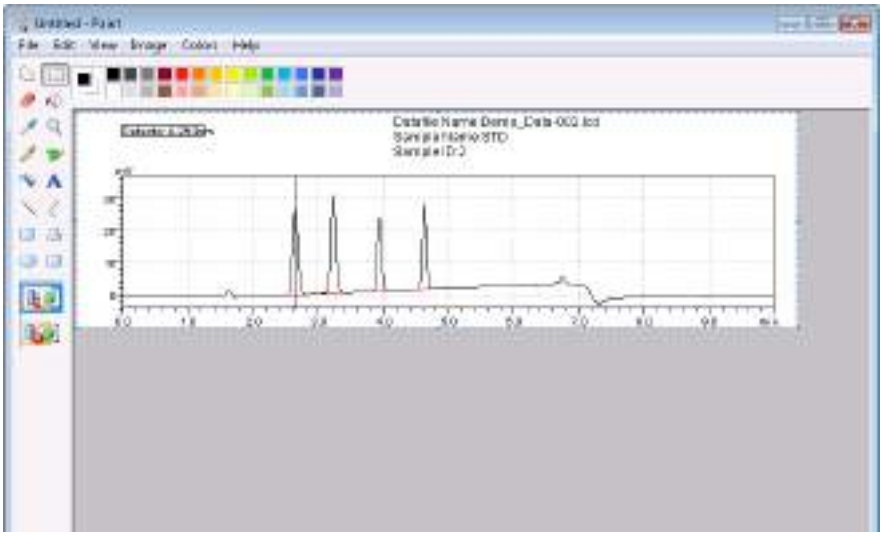
This section describes how to copy chromatograms and Calculation Results Tables displayed in the [Data Analysis] window.

### ■ Copy Chromatograms to the Clipboard

Right-click on the graph in [Chromatogram View], and click [Copy]. The currently displayed content of the chromatogram is copied to the Clipboard.



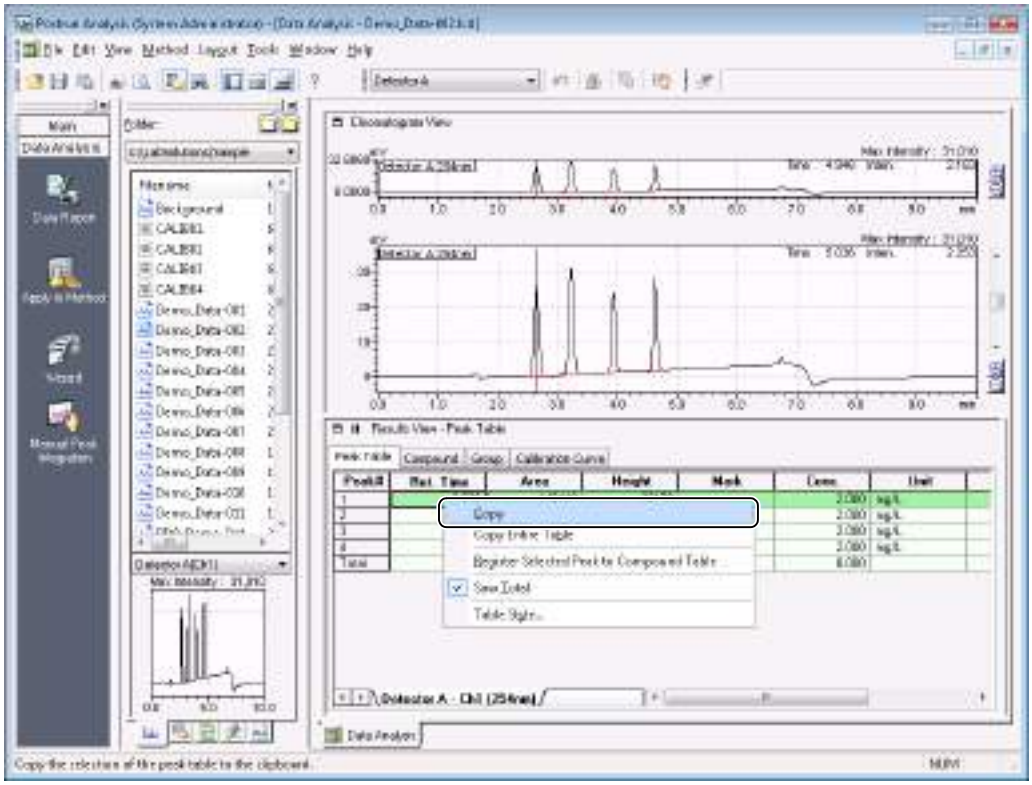
The chromatogram is displayed as follows when it is pasted from the Clipboard to other applications (In this example Paint is used).



## ■ Copy Results Tables to the Clipboard

Select and right-click on the cell or row of a Compound Table or Peak Table, and click [Copy]. The currently displayed table information is copied to the Clipboard.

Click [Copy Entire Table] to copy all of the information included in the table (displayed and hidden).



# 15.3 Common File Operations

The contents of the files displayed in the [Data Explorer] sub-window can be displayed by double-clicking the files in the [Data Explorer] sub-window or dragging-and-dropping them onto each window.

This section describes how to open files in this software.

## 15.3.1 Double-Click Files in the [Data Explorer] Sub-window

This section describes the action when a file in the [Data Explorer] sub-window is double-clicked.

### ■ If the File Display Window Is Not Open

| File Name | Program Name | Open Window |
|---|---|---|
| Method file | [Realtime Analysis] program | [Data Acquisition] window |
| | [Offline Editor] program | [Method Editor] window |
| | [Postrun Analysis] program | [Calibration Curve] window<br>• If the method file contains calibration curve information, all data files for the standard samples that make up the calibration curve are loaded in the [Data Files] tree view. |
| | [Browser] program | [Quant Browser] window<br>• If the method file contains calibration curve information, all standard sample data files that make up the calibration curve are loaded in the [Quantitative Results View]. |
| Data file | [Realtime Analysis] program | [MS Data Analysis] window<br>• The [MS Data Analysis] window opens when data acquisition was performed by a MS detector.<br>[Data Analysis] window<br>[PDA Data Analysis] window<br>• The [PDA Data Analysis] window opens when data acquisition was performed by a photodiode array detector. |
| | [Offline Editor] program | |
| | [Postrun Analysis] program | |
| | [Browser] program | [Data Browser] window<br>• The data file is loaded in the MS chromatogram cell in the [Data Browser] window. |
| Batch file | [Realtime Analysis] program | [Realtime Batch] window |
| | [Offline Editor] program | [Batch Editor] window |
| | [Postrun Analysis] program | [Postrun Batch] window |
| | [Browser] program | [Quant Browser] window<br>• The method file in the initial row of the Batch Table and all data files in the Batch Table open at the same time. |
| Report format file | [Realtime Analysis] program | [Report] window |
| | [Offline Editor] program | |
| | [Postrun Analysis] program | |
| | [Browser] program | |

**NOTE**

- The windows for each of the files are opened from the program according to the file relationships set during installation.
- Double-click a file to load the file in the window indicated in the “Open Window” column.
  If the window is already open, the file is loaded to that window.

## ■ If the File Display Window Is Open

| File Name | Double-Clicked File Handling Window |
|---|---|
| Method file | [Data Acquisition] window |
| | [Method Editor] window |
| | [Calibration Curve] window<br>• If the method file contains calibration curve information, all data files for the standard samples that make up the calibration curve are loaded to the [Data Files] tree view. |
| | [Quant Browser] window<br>• If the method file contains calibration curve information, all standard sample data files that make up the calibration curve are loaded to [Quantitative Results View]. |
| Data file | [MS Data Analysis] window<br>• The [MS Data Analysis] window opens when data acquisition was performed by a MS detector.<br>[Data Analysis] window<br>[PDA Data Analysis] window<br>• The [PDA Data Analysis] window opens when data acquisition was performed by a photodiode array detector. |
| | [Data Comparison] window |
| | [Data Browser] window |
| | [Quant Browser] window<br>• If the method file is not open in the [Quant Browser] window, the method file used to process the data files opens at the same time.<br>• If the method file contains calibration curve information, all data files for the standard samples that make up the calibration curve are loaded to the [Data Files] tree view. |
| Batch file | [Realtime Batch] window |
| | [Batch Editor] window |
| | [Postrun Batch] window |
| | [Quant Browser] window<br>• The method file in the initial row of the Batch Table and all data files in the Batch Table open at the same time. |
| Report format file | [Report] window |

**NOTE**

An exclusive [Report] window for opens for displaying data report format data.

## 15.3.2 Drag-and-Drop Files from the [Data Explorer] Sub-Window

The following table describes the operations equivalent to drag-and-drop to display the method file in a specific window.

### ■ Operations Equivalent To Drag-and-Drop

| File Name | Drop Destination Window | Operations Equivalent to Dragging-and-Dropping |
|---|---|---|
| Method file | [Data Acquisition] window | [File] - [Open Method File] |
| | [Method Editor] window | |
| | [Calibration Curve] window | |
| | [Quant Browser] window | |
| | [MS Data Analysis] window | [File] - [Load Method Parameters]<br>• Default method parameter are set when the method file data does not match the instrument configuration. |
| | [Data Analysis] window | |
| | [PDA Data Analysis] window | |
| Data file | [MS Data Analysis] window | [File] - [Open Data File] |
| | [Data Analysis] window | |
| | [PDA Data Analysis] window | |
| | [Data Comparison] window | [File] - [Open] - [Add Data File] |
| | [Data Browser] window | [File] - [Load Data to Cell] |
| | [Calibration Curve] window | [Data] - [Add]<br>• The data file is displayed in the [Data Files] tree view. |
| | [Quant Browser] window | [Data] - [Add]<br>• If the method file is not open in the [Quant Browser] window, the method file used to process the data file opens at the same time. |
| | [Postrun Batch] window | [Edit] - [Add Rows with Selected Data File] |
| | [Report] window | [File] - [Load Data File] |
| Batch file | [Realtime Batch] window | [File] - [Open Batch File] |
| | [Batch Editor] window | |
| | [Postrun Batch] window | |
| | [Quant Browser] window | [File] - [Load from Batch File]<br>• The method file in the initial row of the Batch Table and all data files in the Batch Table open at the same time. |
| Report format file | [Report] window | [File] - [Open Report Format File] |
| Library file | [UV Library Editor] window | [File] - [Open Library File] |
| | [MS Library Editor] window | |
| Browsing file | [Quant Browser] window | [Layout] - [Open Browsing File]<br>• The method file and data files in the browsing file open at the same time. |
| Layout file | [Data Browser] window | [Layout] - [Open Layout File] |

**NOTE**

- Only the currently displayed data can be displayed in the exclusive [Report] window.
- The method file cannot be opened in a [Calibration Curve] window opened from the [Quant Browser] window.

## ■ Drag-and-Drop Onto a Report with the [Shift] Key Held Down

The following table describes the action when a file is dragged-and-dropped from the [Data Explorer] sub-window onto a report item with the [Shift] key held down.

| File Name | Drop Destination Item | Action |
|---|---|---|
| Method file | [System Configuration] | The system configuration information in the method file is displayed. |
| | [Method] | The instrument parameters and data processing parameters in the method file are displayed. |
| | [Calibration Curve]<br>[MS Calibration Curve] | The calibration curve information in the method file is displayed. |
| Data file | All places where data files can be loaded | Items are displayed individually. The chromatogram of the standard sample and the chromatograms of unknown samples can be displayed in a single report by dropping data files onto each item.<br>**NOTE**<br>• Multiple data files can be dragged-and-dropped onto the [Summary (Concentration)], [Summary (Compound)], [Summary (Data)], [MS Summary (Concentration)], [MS Summary (Compound)], and [MS Summary (Data)] items.<br>• Data files cannot be loaded in the [Line], [Arrow], [Rectangle], [Ellipse], [Picture], and [UV Library] items. |
| Batch file | [Batch Table] | The table and batch table information are displayed.<br>**NOTE**<br>Batch files saved in text format cannot be loaded. |
| Library file | [UV Library] | The spectrum information in the library file is displayed. |
| System check result file | [System Check] | Displays the results of the system check. |

## 15.3.3 Batch Table File Operations

This section describes the action when each cell in the method file, data files and report format files set to the Batch Table are clicked with the [Alt] key on your keyboard held down.

| File Name | Program Name | Open Window |
|---|---|---|
| Method file | [Realtime Analysis] program | [Data Acquisition] window |
| | [Offline Editor] program | [Method Editor] window |
| | [Postrun Analysis] program | [Calibration Curve] window<br>• If the method file contains calibration curve information, all data files for the standard samples that make up the calibration curve are loaded to the [Data Files] tree view. |
| Data file | [Realtime Analysis] program | [MS Data Analysis] window<br>• The [MS Data Analysis] window opens when data acquisition was performed by a MS detector.<br>[Data Analysis] window<br>[PDA Data Analysis] window<br>• If data acquisition was performed with a photodiode array detector, the [PDA Data Analysis] window opens. |
| | [Offline Editor] program | |
| | [Postrun Analysis] program | |
| Report format file | [Realtime Analysis] program | [Report] window |
| | [Offline Editor] program | |
| | [Postrun Analysis] program | |

**NOTE**

While performing an operation on a file in the Batch Table, either select the file with the [Alt] key held down or double-click the file. To make changes, select [Options] on the [Tools] menu, and enter the changes on the [Batch Table Edit] tab in the [Setting Options] sub-window that opens.

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